STATE UNIVERSITY OF NEW YORK AT BUFFALO

JOHANNES KEPLER UNIVERSITY LINZ

Spin-dependency of Linear Response for Particle-Hole Pair Interactions in Fermi Sea and Bosonic System

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A thesis submitted in partial fulfillment for the
Austrian Marshall Plan Program

March 2019

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Abstract

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The effect of spin to the linear response of the system is studied in this paper, with the use of time-dependent Hartree-Fock(TDHF) method and random phase approximation(RPA), for both fermi sea, and bosons under the effect of Rashba coupling. Also, as for the calculation of the static structure function, we use both collective-mode approximation and numerical calculation, and then make a comparison, mainly for the 1-dimensional Rashba bosons. The derivation of TDHF equations is shown in chapter 1, following the steps of Kerman least action principle[1]. And similar steps are follow for the derivation of spin-orbit coupling in fermi sea, as long as the central potential in Rashba bosons. We can see the spin part of fermi sea does not play an important role, even with a spin-dependent interaction. However, as the spin-part is a function of momentum in Rashba bosons, it plays an important role even with a spin-independent interaction. It turns out that the spin splitting of the Rashba bosons makes the Jastrow-Feenberg theory not work any more, as can be see in our comparison of collective-mode methods and numerical result.

Acknowledgements

I would like to thank my sincere friend, host supervisor, Univ. Prof. Robert Zillich, for his introduction of recent topics in cold atoms, and for his help to my settlement and some details in programming. One of Robert's students, Clemens Slaudinger, is also a sincere friend I should never forget.

Above all these people, I am so grateful to Austrian Marshall Plan Foundation, for their support to my study in Austria. Without this, there is no chance for me to have such an unforgettable experience, and I may not have much progress in my research. The host university, Johannes Kepler University Linz, also play a very important role by hosting this project. All the stuffs, especially the secretary of the international office, are so respectable by helping my daily life in JKU Linz.

At the end of the day, the recommandation to this project of my own advisor, SUNY Distinguished Prof. Eckhard Krotscheck, is another main reason why I got the chance of doing research in this place.

Contents

Chapter 1

Introduction

Pairing and correlation phenomena in many-particle systems has been studied in condensed matter physics for many years, however, it remains a main research area in nowadays study, especially when topological materials and high-temperature superconductors become frontier studies. The famous pairing phenomenon in condensed matter physics is the electron-electron pairing in superconductivity, which is well-known as "copper pair". It is the basic requirement of the BCS theory, which is introduced by J.Bardeen, L.Cooper and J.R.Schrieffer in 1957[2]. The BCS theory is very successful in explaining superconductivity in very low temperature, however, it remains a big challenge for its application to high-temperature condition. Therefore, researchers are now looking for a new way to reformulate BCS theory, or new pairing or even higher order correlation phenomena in high temperature superconductivity. A similar challenge is met in recently found graphene "magic angle" by Y.Cao et al.[3]. Therefore, pairing and correlation phenomena will still be a frontier topic in the future.

The widely used pairing phenomenon in condensed matter physics is the electron-hole pair, more generally, the particle-hole pair. It describes the correlation of an excited particle with its original location in the ground state, and is successfully used in solid-state physics. While in solid state we study the pairing of electron with its hole, which is a fermi system, recent development in cold atoms sucessfully simulate lattices with laser beams and Rydberg atoms, and can lead to study of both fermi and bose systems with certain lattice forms.

In this paper, effects of two-body interactions for both fermi sea and 1D Rashba bosons are studied. We focused on the particle-hole interactions which come from the particle-hole pair, and consider if the spin dependency plays an important role. In chapter 2, we derived the response function of fermi sea with central interaction, using time-dependent Hartree-Fock(TDHF) method and random phase approximation(RPA). This is a general formula of RPA with central potential that the Bogoliubov formula of the static structure function, also known as static form factor, comes out naturally by making collective-mode approximation of the response function. And then, in chapter 3, we study the effect of spin-orbit interaction in fermi sea, where we can see the original formula of response function for central interaction doesn't not work properly. And certainly we will not get the Bogoliubov formula when deriving our static form factor. A combined interaction, including central part and spin-orbit part is studied after that. Chapter 4 is our main work during the exchange program, which is the study of 1D Rashba bosons with central interaction. A similar derivation is used to derive the RPA form response function. The analytical expression of our static form factor can be derived analytically, though, it's too complicated for us to use. Therefore, we used a numerical method, by writing an rtsafe program to find all the poles of the response function, then calculated the static form factor by theorem of residue. The collective-mode approximation method is also used to calculate the static form factor. And finally we compared the two results.

Chapter 2

Derivation of Linear Response for Central Potential in Fermi Sea

In this chapter, I'm going to derive the time-dependent Hartree-Fock(TDHF) equation, starting from a fully filled Fermi sea $|\Phi_0\rangle = \prod_{h\leq k_F} a_h^\dagger |0\rangle$, using the principle of least action. Then the expression of response function can be shown based on the TDHF equation and random phase approximation. Time-dependent Hartree-Fock(TDHF) theory is firstly used by Ferrell, Ra to calculate nuclear collective oscillations[4]. It can also be used to calculate molecular properties[5]. This chapter is to make a review of the derivation TDHF equations. Useful steps will be given in our derivation.There can be many different ways to derive the response function, and this is the way our group is using.

2.1 Derivation of TDHF Equations

The time-dependent form of the normal state

$$|\Phi_0\rangle = \prod_{h\leq k_F} a_h^\dagger |0\rangle \tag{2.1}$$

can be written as

$$|\Phi(t)\rangle = e^{iE_0 t/\hbar} \exp\left(\sum_{ph} c_{ph}(t) a_p^\dagger a_h\right) |\Phi_0\rangle \,/\text{Norm} \tag{2.2}$$

Now consider a general Hamiltonian

$$H = T + V - H_0 + \delta H \tag{2.3}$$

where H_0 is the ground state Hamiltonian, T is the kinetic energy, V is the interaction part and δH is the perturbation. Generally speaking, the time-dependent Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\left|\Phi(t)\right\rangle = H\left|\Phi(t)\right\rangle \tag{2.4}$$

is not satisfied for the time-dependent normal state. What we can do is to introduce a general Lagrangian

$$L = \left\langle\Phi(t)\right|\left(i\hbar\frac{\partial}{\partial t} - H\right)\left|\Phi(t)\right\rangle \tag{2.5}$$

and a general action

$$S = \int L dt \tag{2.6}$$

then use the principle of least action to let the variation of action

$$\delta S = 0 \tag{2.7}$$

This is the Kerman-Koonin principle[1]. We will see that by the two equations of variational principle,

$$\frac{\delta S}{\delta c_{ph}} = 0, \quad \frac{\delta S}{\delta c^*_{ph}} = 0 \tag{2.8}$$

the TDHF equations can be derived. To achieve this, we need to calculate all the terms in our general Lagrangian. Here we need approximation to 1st order in δH, 2nd order in $H_1 = T + V$, and 1st order in our density operator $\hat{\rho}(\mathbf{r})$, where

$$\hat{\rho}(\mathbf{r}) = \sum_{\alpha\beta}\phi^*_\alpha(\mathbf{r})\phi_\beta(\mathbf{r})a^\dagger_\alpha a_\beta \tag{2.9}$$

2.1.1 Normalization of the state

First we need to consider the normalization $\langle\Phi(t)|\Phi(t)\rangle$. The exponential term part of time dependency gives us infinite order of $c_{ph}a^\dagger_p a_h$. In our calculation, we just need 1st-order approximation of our state, which will give us 2nd-order of mean value. So

$$\begin{aligned}
&\left\langle\Phi_0\right| e^{\sum_{ph} c^*_{ph}a^\dagger_h a_p} e^{\sum_{ph} c_{ph}a^\dagger_p a_h}\left|\Phi_0\right\rangle \\
=&\left\langle\Phi_0|\Phi_0\right\rangle + \sum_{ph}\left\langle\Phi_0\right| a^\dagger_h a_p\left|\Phi_0\right\rangle c^*_{ph} + \text{c.c} + \sum_{pp'hh'} c_{ph}c^*_{p'h'}\left\langle\Phi_0\right| a^\dagger_{h'}a_{p'}a^\dagger_p a_h\left|\Phi_0\right\rangle \\
=&1 + \sum_{ph}\left|c_{ph}\right|^2
\end{aligned} \tag{2.10}$$

The second term and the third term in the intermediate step vanish because we assumed $p > k_F$.

2.1.2 Time-derivative term

Recall that

$$|\Phi(t)\rangle = \frac{e^{-iE_0t/\hbar}e^{\sum c_{ph}(t)a_p^\dagger a_h}|\Phi_0\rangle}{\langle\Phi_0|e^{\sum c_{ph}^* a_h^\dagger a_p}e^{\sum c_{ph}a_p^\dagger a_h}|\Phi_0\rangle^{1/2}} = e^{-iE_0t/\hbar}|\Phi_0(t)\rangle \tag{2.11}$$

so

$$\begin{aligned}
&\langle\Phi(t)| - i\hbar\frac{\partial}{\partial t}|\Phi(t)\rangle = -E_0 + \langle\Phi_0(t)| - i\hbar\frac{\partial}{\partial t}|\Phi_0(t)\rangle \\
=& -E_0 - i\hbar\langle\Phi_0(t)|\sum_{ph}\dot{c}_{ph}a_p^\dagger a_h|\Phi_0(t)\rangle + \frac{1}{2}i\hbar\langle\Phi_0(t)|\sum_{ph}(\dot{c}_{ph}a_p^\dagger a_h + \dot{c}_{ph}^* a_h^\dagger a_p)|\Phi_0(t)\rangle \\
=& -E_0 - \frac{i}{2}\hbar\langle\Phi_0(t)|\sum_{ph}(\dot{c}_{ph}a_P^\dagger a_h - \dot{c}_{ph}^* a_h^\dagger a_p)|\Phi_0(t)\rangle \\
=& -E_0 - \frac{i}{2}\sum_{pp'hh'}\Big[\langle\Phi_0|c_{p'h'}^* a_{h'}^\dagger a_{p'}(\dot{c}_{ph}a_p^\dagger a_h - \dot{c}_{ph}^* a_h^\dagger a_p) + (\dot{c}_{ph}a_p^\dagger a_h - \dot{c}_{ph}^* a_h^\dagger a_p)c_{p'h'}a_{p'}^\dagger a_{h'}|\Phi_0\rangle\Big] \\
=& -E_0 + \frac{i}{2}\hbar\sum_{ph}[\dot{c}_{ph}^* c_{ph} - \dot{c}_{ph}c_{ph}^*]
\end{aligned} \tag{2.12}$$

2.1.3 Perturbation term

The perturbation operator can be written as

$$\delta H = \sum_{\alpha\beta}\langle\alpha|\delta H|\beta\rangle a_\alpha^\dagger a_\beta \tag{2.13}$$

So

$$\begin{aligned}
\langle\Phi(t)|\delta H|\Phi(t)\rangle &= \sum_{\alpha\beta ph}\Big[\langle\Phi_0|c_{ph}^* a_h^\dagger a_p a_\alpha^\dagger a_\beta|\Phi_0\rangle + \langle\Phi_0|a_\alpha^\dagger a_\beta c_{ph}a_p^\dagger a_h|\Phi_0\rangle]\langle\alpha|\delta H|\beta\rangle \\
&= \sum_{ph}[c_{ph}^*\langle p|\delta H|h\rangle + c_{ph}\langle h|\delta H|p\rangle]
\end{aligned} \tag{2.14}$$

Here the perturbation is assumed to contain only non-diagonal terms.

2.1.4 Density

From the eq.(2.9) of density operator, we can calculate the time-denpendent form of density

$$\begin{aligned}\rho(\mathbf{r},t) = \langle\Phi(t)|\,\hat{\rho}(\mathbf{r})\,|\Phi(t)\rangle = \sum_{\alpha\beta}\langle\Phi_0|\,(1+\sum_{ph}c^*_{ph}a^\dagger_h a_p)a^\dagger_\alpha a_\beta(1+\sum_{ph}c_{ph}a^\dagger_p a_h)\,|\Phi_0\rangle\,\phi^*_\alpha\phi_\beta \\ =&\rho(\mathbf{r}) + \sum_{\alpha\beta}\phi^*_\alpha(\mathbf{r})\phi_\beta(\mathbf{r})\,\langle\Phi_0|\,(c^*_{ph}a^\dagger_h a_p a^\dagger_\alpha a_\beta + c_{ph}a^\dagger_\alpha a_\beta a^\dagger_p a_h)\,|\Phi_0\rangle \\ =&\rho(\mathbf{r}) + \sum_{ph}[c^*_{ph}\phi^*_p(\mathbf{r})\phi_h(\mathbf{r}) + c_{ph}\phi^*_h(\mathbf{r})\phi_p(\mathbf{r})] \\ =&\rho(\mathbf{r}) + \delta\rho(\mathbf{r},t)\end{aligned} \tag{2.15}$$

The second term,

$$\delta\rho(\mathbf{r},t) = \langle\Phi_0|\,\hat{\rho}\,|\delta\Phi\rangle + \langle\delta\Phi|\,\hat{\rho}\,|\Phi_0\rangle \tag{2.16}$$

is called transition density. We need to use this term to derive the response function. Here

$$|\delta\Phi\rangle = \sum_{ph}c_{ph}a^\dagger_p a_h\,|\Phi_0\rangle \tag{2.17}$$

2.1.5 Non-perturbative Hamiltonian $H_1 - H_0$

The mean value of the non-perturbative Hamiltonian is

$$\frac{\langle\Phi_0|\,e^{\sum c^*_{ph}a^\dagger_h a_p}(H_1-H_0)e^{\sum c_{ph}a^\dagger_p a_h}\,|\Phi_0\rangle}{\langle\Phi_0|\,e^{\sum c^*_{ph}a^\dagger_h a_p}e^{\sum c_{ph}a^\dagger_p a_h}\,|\Phi_0\rangle} \tag{2.18}$$

Now take a look at the 1st-order terms,

$$\sum_{ph}c_{ph}\,\langle\Phi_0|\,(H_1-H_0)\left|a^\dagger_p a_h\Phi_0\right\rangle = \text{c.c} = 0 \tag{2.19}$$

This is actually the Brillouin condition. We can then calculate the 2nd-order terms. Here we don't need the denominator because the numerator is 2nd-order.

$$\begin{aligned}&\langle\Phi_0|\,\frac{1}{2!}\left(\sum_{ph}c^*_{pp'hh'}c^*_{p'h'}a^\dagger_h a_p a^\dagger_{h'}a_{p'}\right)(H_1-H_0)\,|\Phi_0\rangle \\ &+\langle\Phi_0|\sum_{ph}c^*_{ph}a^\dagger_h a_p(H_1-H_0)\sum_{p'h'}c_{p'h'}a^\dagger_{p'}a_{h'}\,|\Phi_0\rangle \\ &+\frac{1}{2!}\,\langle\Phi_0|\,(H_1-H_0)\left(\sum_{ph}c^*_{pp'hh'}c^*_{p'h'}a^\dagger_h a_p a^\dagger_{h'}a_{p'}\right)|\Phi_0\rangle\end{aligned} \tag{2.20}$$

We can then calculate term by term. Notice that all the H_0 term will vanish. Then we can take a look the third term, which is the Hermitian conjugate of the first term so they will have similar results.

$$
\begin{aligned}
&\langle\Phi_0|(H_1-H_0)a_p^\dagger a_h a_{p'}^\dagger a_{h'}|\Phi_0\rangle = \sum_{\alpha\beta}\sum_{pp'hh'}\langle\alpha|(T-H_0)|\beta\rangle\langle\Phi_0|a_\alpha^\dagger a_\beta a_p^\dagger a_h a_{p'}^\dagger a_{h'}|\Phi_0\rangle \\
&+\frac{1}{4}\sum_{\alpha\beta\gamma\delta}\sum_{pp'hh'}\langle\alpha\beta|V|\gamma\delta\rangle\langle\Phi_0|a_\alpha^\dagger a_\beta^\dagger a_\delta a_\gamma a_p^\dagger a_h a_{p'}^\dagger a_{h'}|\Phi_0\rangle \\
&=\frac{1}{4}\sum_{\alpha\beta}\langle\alpha\beta|V|p'p\rangle_a\langle\Phi_0|a_\alpha^\dagger a_\beta^\dagger a_h a_{h'}|\Phi_0\rangle \\
&=\frac{1}{2}\sum_{pp'hh'}\langle hh'|V|pp'\rangle_a
\end{aligned}
\tag{2.21}
$$

For the second term, following similar calculations

$$
\langle\Phi_0|a_h^\dagger a_p(H_1-H_0)a_{p'}^\dagger a_{h'}|\Phi_0\rangle = \sum_{pp'hh'}[(\varepsilon_{p'}-\varepsilon_{h'})\delta_{pp'}\delta_{hh'}+\langle ph'|V|hp'\rangle_a] \tag{2.22}
$$

2.1.6 Lagrangian and Euler equation

Now we can write down the expression of our general Hamiltonian,

$$
\begin{aligned}
L =&\frac{1}{2}\sum_{pp'hh'}\{c_{ph}c_{p'h'}\langle hh'|V|pp'\rangle_a + c_{ph}^* c_{p'h'}^*\langle pp'|V|hh'\rangle_a \\
&+2c_{ph}c_{p'h'}^*[(\varepsilon_{p'}-\varepsilon_{h'})\delta_{pp'}\delta_{hh'}+\langle ph'|V|hp'\rangle]\} \\
&-\frac{i\hbar}{2}\sum_{ph}[c_{ph}^*\dot{c}_{ph}-c_{ph}\dot{c}_{ph}^*] \\
&+\sum_{ph}[c_{ph}^*\langle p|\delta H|h\rangle + c_{ph}\langle h|\delta H|p\rangle]
\end{aligned}
\tag{2.23}
$$

From eq.(2.8) we can get the Euler equations

$$
\sum_{p'h'}\{\langle pp'|V|hh'\rangle c_{p'h'}^* + [(\varepsilon_p-\varepsilon_h)\delta_{pp'}\delta hh' + \langle ph'|V|hp'\rangle_a]c_{p'h'}\} + \langle p|\delta H|h\rangle = i\hbar\dot{c}_{ph} \tag{2.24}
$$

$$
\sum_{p'h'}\{\langle hh'|V|pp'\rangle c_{p'h'} + [(\varepsilon_p-\varepsilon_h)\delta_{pp'}\delta hh' + \langle ph'|V|hp'\rangle_a]c_{p'h'}^*\} + \langle h|\delta H|p\rangle = -i\hbar\dot{c}_{ph}^* \tag{2.25}
$$

Here we can use the supermatrix notation to define

$$
\mathbf{A} = (A_{pp'hh'}) = [(\varepsilon_p-\varepsilon_h)\delta_{pp'}\delta_{hh'}+\langle ph'|V|hp'\rangle_a] \tag{2.26}
$$

$$
\mathbf{B} = (B_{pp'hh'}) = \langle pp'|V|hh'\rangle_a \tag{2.27}
$$

$$
\mathbf{c} = (c_{ph}) \tag{2.28}
$$

The Euler equations can then be written in supermatrix form

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^{\dagger} & \mathbf{A}^{\dagger} \end{pmatrix} \begin{pmatrix} c \\ c^{*} \end{pmatrix} + \begin{pmatrix} \delta H \\ \delta H^{*} \end{pmatrix} = i\hbar \frac{d}{dt} \begin{pmatrix} c \\ -c^{*} \end{pmatrix} \tag{2.29}$$

Let $c = xe^{-i\omega t} + y^{*}e^{i\omega t}$, we get

$$\begin{pmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{B}^{\dagger} & \mathbf{A}^{\dagger} \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} \delta H \\ \delta H^{*} \end{pmatrix} = \hbar\omega \begin{pmatrix} x \\ -y \end{pmatrix} \tag{2.30}$$

This supermatrix eqution is our TDHF equation.

2.2 Random Phase Approximation

We can now derive the response function using random phase approximation. In this approximation, we assume an infinite system limit, and ε_p, ε_h are approximated to free spectrum. Also, we omit exchange interaction so the antisymmetric terms $\langle ph'| V |hp'\rangle_a$ and $\langle pp'| V |hh'\rangle_a$ will reduce to $\langle ph'| V |hp'\rangle$ and $\langle pp'| V |hh'\rangle$. We can then calculate these two terms in plane-wave basis.

$$\begin{aligned}
\langle ph'| V |hp'\rangle &= \frac{1}{\Omega^2} \int d^3r_1 d^3r_2 V(|\mathbf{r}_1 - \mathbf{r}_2|) e^{-i\mathbf{p}\cdot\mathbf{r}_1 - i\mathbf{h}'\cdot\mathbf{r}_1 + i\mathbf{h}\cdot\mathbf{r}_2 + i\mathbf{p}'\cdot\mathbf{r}_2} \\
&= \frac{1}{\Omega^2} \int d^3r_1 d^3r_2 V(|\mathbf{r}_1 - \mathbf{r}_2|) e^{-i(\mathbf{p}+\mathbf{h})\cdot(\mathbf{r}_1-\mathbf{r}_2) + i(-\mathbf{p}-\mathbf{h}'+\mathbf{h}+\mathbf{p}')\cdot\mathbf{r}_2} \\
&= \frac{1}{\Omega}\delta(\mathbf{p}+\mathbf{h}'-\mathbf{h}-\mathbf{p}') \int d^3r_{12} V(|\mathbf{r}_1 - \mathbf{r}_2|) e^{-i(\mathbf{p}-\mathbf{h})\cdot\mathbf{r}_{12}} \\
&= \delta(\mathbf{p}+\mathbf{h}'-\mathbf{h}-\mathbf{p}') \frac{1}{N} \tilde{V}(|\mathbf{p}-\mathbf{h}|) \\
&= \frac{1}{N}\tilde{V}(q)\delta(\mathbf{q}-\mathbf{q}')
\end{aligned} \tag{2.31}$$

Here we let $\mathbf{p} - \mathbf{h} = \mathbf{q}$, $\mathbf{p}' - \mathbf{h}' = \mathbf{q}'$. Follow similar calculations we can also get

$$\langle pp'| V |hh'\rangle = \frac{1}{N}\tilde{V}(q)\delta(\mathbf{q}+\mathbf{q}') \tag{2.32}$$

$$\langle p| \delta H |h\rangle = \delta\tilde{H}(q) \tag{2.33}$$

So we will have

$$Ax_{ph} = (\varepsilon_p - \varepsilon_h)x_{ph} + \sum p'h'\tilde{V}(q)\frac{1}{N}\delta_{\mathbf{p}',\mathbf{h}'+\mathbf{q}}x_{p'h'} \tag{2.34}$$

$$= (\varepsilon_p - \varepsilon_h)x_{ph} + \tilde{V}(q)\tilde{x}(q) \tag{2.35}$$

$$By_{ph} = \sum_{p'h'} \frac{1}{N}\tilde{V}(q)\delta_{\mathbf{p}',\mathbf{h}'-\mathbf{q}}y_{p'h'} = \tilde{V}(q)\tilde{y}(q) \tag{2.36}$$

Here we let

$$\tilde{x}(q) = \frac{1}{N}\sum_{h'} x_{h'+q,h'} \tag{2.37}$$

$$\tilde{y}(q) = \frac{1}{N}\sum_{h'} y_{h'-q,h'} \tag{2.38}$$

Notice that since $x_{p'h'}$ and $y_{p'h'}$ depend only on the magnitue p' and h', we can expect that

$$\sum_{h'} x_{h'+q,h'} = \sum_{h'} x_{h'-q,h'} \tag{2.39}$$

$$\sum_{h'} y_{h'-q,h'} = \sum_{h'} y_{h'+q,h'} \tag{2.40}$$

because for a certain $\mathbf{h}' + \mathbf{q}$ we can always find the inverse direction of $\mathbf{h}'$ to get $-\mathbf{h}' - \mathbf{q}$, which has the same amplitude. So the total sum will be the same. Now the supermatrix equation can be written as

$$(\varepsilon_p - \varepsilon_h - \omega)x_{ph} + \tilde{V}(q)[\tilde{x}(q) + \tilde{y}(q)] + \delta\tilde{H}(q) = 0 \tag{2.41}$$

$$(\varepsilon_p - \varepsilon_h + \omega)y_{ph} + \tilde{V}(q)[\tilde{x}(q) + \tilde{y}(q)] + \delta\tilde{H}(q) = 0 \tag{2.42}$$

And these two equation can be reformualted to

$$\tilde{x}(q) = -\left[\frac{1}{N}\sum_{h}\frac{1}{\varepsilon_p - \varepsilon_h - \omega}\right]\left[\tilde{V}(q)[\tilde{x} + \tilde{y}] + \delta\tilde{H}\right] \tag{2.43}$$

$$\tilde{y}(q) = -\left[\frac{1}{N}\sum_{h}\frac{1}{\varepsilon_p - \varepsilon_h + \omega}\right]\left[\tilde{V}(q)[\tilde{x} + \tilde{y}] + \delta\tilde{H}\right] \tag{2.44}$$

Now we can get

$$\delta\tilde{\rho}(q) = \tilde{x}(q) + \tilde{y}(q) = \frac{\chi_0(q,\omega)}{1 - \tilde{V}(q)\chi_0(q,\omega)}\delta\tilde{H}(q) \tag{2.45}$$

So the response function is

$$\chi(q,\omega) = \frac{\chi_0(q,\omega)}{1 - \tilde{V}(q)\chi_0(q,\omega)} \tag{2.46}$$

Here

$$\chi_0 = -\frac{1}{N}\sum_{h}\left(\frac{1}{\varepsilon_p - \varepsilon_h - \omega} + \frac{1}{\varepsilon_p - \varepsilon_h + \omega}\right) \tag{2.47}$$

Chapter 3

Spin-Orbit Coupling in Fermi Sea

In this chapter, we will follow similar steps from Chapter 1 to derive the response function fo spin-orbit coupling in fermi sea. The difference here is the interaction includes not only spatial part, but also spin part and orbital part. Therefore, we should consider the spin dependency in our state. Here we will consider only the orbital part first in our interaction, then take into account the spin part to see if it generates any differences.

3.1 Derivation of Response Function

Now we can consider a spin-orbit coupling in the form

$$V = V(r)\mathbf{L} \cdot \mathbf{S} = V(r)\mathbf{r} \times \mathbf{p} \cdot \mathbf{S} \tag{3.1}$$

Since the spins are randomly distrubuted and we don't know the exact spin direction of a certain particle, we can treat the spin operator as the mean value of all matrix elements in the total spin operator. Let's define it as $\mathbf{s}$, it should remain the same in our two-body interaction that

$$\mathbf{s} = \sum_{\sigma_p \sigma_{p'} \sigma_h \sigma_{h'}} \left\langle \sigma_p \sigma_{p'} \right| \mathbf{S} \left| \sigma_h \sigma_{h'} \right\rangle = \sum_{\sigma_p \sigma_{p'} \sigma_h \sigma_{h'}} \left\langle \sigma_p \sigma_{h'} \right| \mathbf{S} \left| \sigma_h \sigma_{p'} \right\rangle \tag{3.2}$$

and will not affect the form of our response function. So now we can consider only the orbital part $V(r)\mathbf{r} \times \mathbf{p}$. The only thing changed in our TDHF equations is the interaction part. Now we can calculated them in plane-wave basis. Notice that for a two-body interaction, our interaction form should be written as

$$V = V(|\mathbf{r}_1 - \mathbf{r}_2|)\mathbf{r}_{12} \times \mathbf{p}_{12} \tag{3.3}$$

Here $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$, $\mathbf{p}_{12} = \frac{1}{2}(\mathbf{p}_1 - \mathbf{p}_2)$. Following similar calculations in plane-wave basis, we will get

$$\langle ph' | V | hp' \rangle = \frac{i}{2N}\delta(\mathbf{p} + \mathbf{h}' - \mathbf{h} - \mathbf{p}')\nabla_{\mathbf{q}}\tilde{V}(q) \times (\mathbf{h} - \mathbf{p}') \tag{3.4}$$

We can further simplify it by $\nabla_{\mathbf{q}}\tilde{V}(q) = \tilde{V}'(q)\hat{q}$ that

$$\langle ph' | V | hp' \rangle = \frac{i}{2N}\delta(\mathbf{q} - \mathbf{q}')\tilde{V}'(q)\hat{q} \times (\mathbf{h} - \mathbf{h}') \tag{3.5}$$

Similarly we can get

$$\langle pp' | V | hh' \rangle = \frac{i}{2N}\delta(\mathbf{q} + \mathbf{q}')\tilde{V}'(q)\hat{q} \times (\mathbf{h} - \mathbf{h}') \tag{3.6}$$

Now the TDHF equations will become

$$\begin{aligned}(\varepsilon_p - \varepsilon_h - \omega)x_{ph} + \frac{i}{2N}\frac{\partial \tilde{V}}{\partial q}\sum_{p'h'}\big[(\delta(\mathbf{p} + \mathbf{h}' - \mathbf{h} - \mathbf{p}')\hat{q} \times (\mathbf{h} - \mathbf{h}')x_{p'h'} \\ + \delta(\mathbf{p} + \mathbf{p}' - \mathbf{h} - \mathbf{h}')\hat{q} \times (\mathbf{h} - \mathbf{h}')y_{p'h'}\big] + \delta\tilde{H}(q) = 0 \\ (\varepsilon_p - \varepsilon_h + \omega)y_{ph} + \frac{-i}{2N}\frac{\partial \tilde{V}}{\partial q}\sum_{p'h'}\big[(\delta(\mathbf{p} + \mathbf{p}' - \mathbf{h} - \mathbf{h}')\hat{q} \times (\mathbf{h} - \mathbf{h}')x_{p'h'} \\ + \delta(\mathbf{p} + \mathbf{h}' - \mathbf{h} - \mathbf{p}')\hat{q} \times (\mathbf{h} - \mathbf{h}')y_{p'h'}\big] + \delta\tilde{H}(q) = 0\end{aligned} \tag{3.7}$$

Follow similar analysis we have

$$\begin{aligned}\sum_{h'}\mathbf{h}'x_{h'-q,h'} &= -\sum_{h'}\mathbf{h}'x_{h'+q,h'} \\ \sum_{h'}\mathbf{h}'y_{h'-q,h'} &= -\sum_{h'}\mathbf{h}'y_{h'+q,h'}\end{aligned} \tag{3.8}$$

Now we define four terms

$$\begin{aligned}\tilde{x}(q) &= \frac{1}{N}\sum_{h'}x_{h'+q,h'} \\ \tilde{x'}(q) &= \frac{1}{N}\hat{q} \times \sum_{h'}\mathbf{h}'x_{h'+q,h'}\end{aligned} \tag{3.9}$$

$$\begin{aligned}\tilde{y}(q) &= \frac{1}{N}\sum_{h'}y_{h'+q,h'} \\ \tilde{y'}(q) &= \frac{1}{N}\hat{q} \times \sum_{h'}\mathbf{h}'y_{h'+q,h'}\end{aligned} \tag{3.10}$$

Then we will have four equations

$$
\begin{aligned}
\tilde{x}(q) &= -\frac{1}{N}\sum_h \frac{1}{\varepsilon_p-\varepsilon_h-\omega}\left[\frac{i}{2}\frac{\partial\tilde{V}}{\partial q}(\hat{q}\times\mathbf{h}(\tilde{x}(q)+\tilde{y}(q))-(\tilde{x'}(q)-\tilde{y'}(q)))+\delta\tilde{H}(q)\right]\\
\tilde{y}(q) &= -\frac{1}{N}\sum_h \frac{1}{\varepsilon_p-\varepsilon_h+\omega}\left[\frac{-i}{2}\frac{\partial\tilde{V}}{\partial q}(\hat{q}\times\mathbf{h}(\tilde{x}(q)+\tilde{y}(q))+(\tilde{x'}(q)-\tilde{y'}(q)))+\delta\tilde{H}(q)\right]\\
\tilde{x'}(q) &= -\frac{1}{N}\hat{q}\times\sum_h \frac{\mathbf{h}}{\varepsilon_p-\varepsilon_h-\omega}\left[\frac{i}{2}\frac{\partial\tilde{V}}{\partial q}(\hat{q}\times\mathbf{h}(\tilde{x}(q)+\tilde{y}(q))-(\tilde{x'}(q)-\tilde{y'}(q)))+\delta\tilde{H}(q)\right]\\
\tilde{y'}(q) &= -\frac{1}{N}\hat{q}\times\sum_h \frac{\mathbf{h}}{\varepsilon_p-\varepsilon_h+\omega}\left[\frac{-i}{2}\frac{\partial\tilde{V}}{\partial q}(\hat{q}\times\mathbf{h}(\tilde{x}(q)+\tilde{y}(q))+(\tilde{x'}(q)-\tilde{y'}(q)))+\delta\tilde{H}(q)\right]
\end{aligned}
\tag{3.11}
$$

Finally we will get our transition density $\delta\tilde{\rho}(q)=\tilde{x}(q)+\tilde{y}(q)$ as

$$
\frac{\chi_0-\frac{i}{2N}\frac{\partial\tilde{V}}{\partial q}\left[\left(\sum_h v(h,\omega)\right)\left(\sum_h \hat{q}\times\mathbf{h}v(h,\omega)\right)-\left(\sum_h v(h,\omega)\right)\left(\sum_h \hat{q}\times\mathbf{h}v(h,\omega)\right)\right]}{1+\frac{1}{4N^2}\left(\frac{\partial\tilde{V}}{\partial q}\right)^2\left(\sum_h \hat{q}\times\mathbf{h}v(h,\omega)\right)^2-\frac{1}{4N^2}\left(\frac{\partial\tilde{V}}{\partial q}\right)^2\left(\sum_h u(h,\omega)\right)\left(\sum_h \hat{q}\times\mathbf{h}u(h,\omega)\hat{q}\times\mathbf{h}\right)}\delta\tilde{H}(q)
\tag{3.12}
$$

Here we defined

$$
u(h,\omega)=\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega} \tag{3.13}
$$

$$
v(h,\omega)=\frac{1}{\varepsilon_p-\varepsilon_h-\omega}-\frac{1}{\varepsilon_p-\varepsilon_h+\omega} \tag{3.14}
$$

And

$$
\chi_0=-\frac{1}{N}\sum_h u(h,\omega) \tag{3.15}
$$

Therefore, our response function for the spin-orbit coupling, including the spin part, defined as $\chi(q,\omega)$, will be

$$
\frac{\chi_0-\frac{i}{2N}\frac{\partial\tilde{V}}{\partial q}\left[\left(\sum_h v(h,\omega)\right)\left(\sum_h(\hat{q}\times\mathbf{h}\cdot\mathbf{s})v(h,\omega)\right)-\left(\sum_h v(h,\omega)\right)\left(\sum_h(\hat{q}\times\mathbf{h}\cdot\mathbf{s})v(h,\omega)\right)\right]}{1+\frac{1}{4N^2}\left(\frac{\partial\tilde{V}}{\partial q}\right)^2\left(\sum_h(\hat{q}\times\mathbf{h}\cdot\mathbf{s})v(h,\omega)\right)^2-\frac{1}{4N^2}\left(\frac{\partial\tilde{V}}{\partial q}\right)^2\left(\sum_h u(h,\omega)\right)\left(\sum_h(\hat{q}\times\mathbf{h}\cdot\mathbf{s})^2u(h,\omega)\right)}
\tag{3.16}
$$

Now we can take a look at the sums $\sum\mathbf{h}u(h,\omega)$ and $\sum\mathbf{h}v(h,\omega)$. The denominators are in the form

$$
\varepsilon_p-\varepsilon_h\pm\omega=\frac{\hbar^2}{2m}[(\mathbf{h}+\mathbf{q})^2-\mathbf{h}^2]\pm\omega=\frac{\hbar^2}{2m}(q^2+2\mathbf{h}\cdot\mathbf{q})\pm\omega \tag{3.17}
$$

It is azimuthally symmetric around the direction of q. So the sums $\sum\mathbf{h}u(h,\omega)$ and $\sum\mathbf{h}v(h,\omega)$ will point to the direction of q. This will make life easier because all the terms containing $\sum\hat{\mathbf{q}}\times\mathbf{h}u(h,\omega)$

and $\sum \hat{\mathbf{q}} \times \mathbf{h} v(h, \omega)$ will vanish. Now our response function will reduce to

$$\chi(q, \omega) = \frac{\chi_0}{1 - \frac{1}{4N^2} \left(\frac{\partial \tilde{V}}{\partial q}\right)^2 \left(\sum_h u(h, \omega)\right) \left(\sum_h (\hat{\mathbf{q}} \times \mathbf{h} \cdot \mathbf{s})^2 u(h, \omega)\right)} = \frac{\chi_0}{1 - \chi^{(2)}} \tag{3.18}$$

And here

$$\chi^{(2)} = \chi_0^{(2)} \chi_1^{(2)} \tag{3.19}$$

$$\chi_0^{(2)} = \sum_h u(h, \omega) \tag{3.20}$$

$$\chi_1^{(2)} = \sum_h (\hat{\mathbf{q}} \times \mathbf{h} \cdot \mathbf{s})^2 u(h, \omega) \tag{3.21}$$

An evaluation of $\chi_1^{(2)}$ is done in Appendix A.

3.2 Collective Mode Approximation

Now we need to calculate the collective mode approximation for spin-orbit coupling. Following similar steps as the case of central potential, we assumed the collective mode of free-particle response function, what is known as Lindhard function, has the form

$$\frac{1}{q^2 + 2\mathbf{q} \cdot \mathbf{h} \pm \omega} \rightarrow \frac{a(q)}{b(q) \pm \omega} \tag{3.22}$$

It also makes the denominator of our Lindhard function independent from the $\sum_h$. Then we will have

$$\chi_0(\mathbf{q}, \omega) = \frac{1}{N} \sum_h \left(\frac{a(q)}{b(q) - \omega} + \frac{a(q)}{b(q) + \omega}\right) = 2\frac{V}{(2\pi)^3 N} \int d^3h \left(\frac{a(q)}{b(q) - \omega} + \frac{a(q)}{b(q) + \omega}\right) \tag{3.23}$$

It's easy to determine $a(q)$ and $b(q)$ from the f-sum rules that $a(q) = 1$, $b(q) = q^2/S_f(q)$, where $S_f(q)$ is the static form factor.

$$S_f(q) = \frac{1}{N} \int S(q, \omega) d\omega = \frac{1}{N} \int \sum_n |(\rho_q^+)_{no}|^2 \delta(\omega_{no} - \omega) d\omega \tag{3.24}$$

For the case $q > 2k_f$, all holes can be excited to particles, so $S_f(q) = 1$. For the case $q \leq 2k_f$,

$$\begin{aligned} S_f(q) &= 2\frac{V}{(2\pi)^3 N} \left(\int_0^{2\pi} d\phi \int_{-q/2}^{k_f} dz \int_0^{\sqrt{k_f^2 - z^2}} d\rho\rho - \int_0^{2\pi} d\phi \int_{-q/2}^{k_f - q} dz \int_0^{\sqrt{k_f^2 - (z+q)^2}} d\rho\rho\right) \\ &= \frac{3}{4k_f^3} \left(k_f^2 q - \frac{q^3}{12}\right) \end{aligned} \tag{3.25}$$

And actually $S_f(q) = \frac{2V}{(2\pi)^3 N}\int d^3h$. Notice here that we use the formula of fermi energy $E_f = \frac{\hbar^2}{2m}(3\pi^2 N/V)^{2/3}$, which gives us $V/N = 3\pi^2/k_f^3$. Also a prefactor 2 is because of the degeneracy of fermions. So following the expression of our calculated response function

$$\chi(q,\omega) = \frac{\frac{1}{N}\sum_h u(h,\omega)}{1 - \frac{1}{4N^2}\left(\frac{\partial\tilde{V}}{\partial q}\right)^2 \left(\sum_h u(h,\omega)\right)\left(\sum_h (\hat{\mathbf{q}}\times\mathbf{h}\cdot\mathbf{s})^2 u(h,\omega)\right)} \tag{3.26}$$

we get

$$\chi^{coll}(q,\omega) = \frac{\frac{1}{b(q)-\omega}+\frac{1}{b(q)+\omega}}{1 - S_f(q)\left(\frac{\partial\tilde{V}}{\partial q}\right)^2\left(\frac{1}{b(q)-\omega}+\frac{1}{b(q)+\omega}\right)^2 \frac{2V}{(2\pi)^3N}\int d^3h(\hat{\mathbf{q}}\times\mathbf{h}\cdot\mathbf{s})^2} \tag{3.27}$$

Now we need to evaluate $(\hat{\mathbf{q}}\times\mathbf{h}\cdot\mathbf{s})^2$ term. Using the formula

$$(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = \mathbf{a}\cdot\mathbf{b}(\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}) - i\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}) = \mathbf{a}\cdot\mathbf{b} - i\boldsymbol{\sigma}\cdot(\mathbf{a}\times\mathbf{b}) \tag{3.28}$$

Here $\mathbf{a} = \mathbf{b} = \hat{\mathbf{q}}\times\mathbf{h}$, $\mathbf{S} = \frac{1}{2}\boldsymbol{\sigma}$. So we have

$$(\hat{\mathbf{q}}\times\mathbf{h}\cdot\mathbf{S})^2 = \frac{1}{4}(\hat{\mathbf{q}}\times\mathbf{h})^2\cdot I = \frac{1}{4}h^2\sin^2\theta\cdot I \tag{3.29}$$

Now we can consider the sum of all spin distribution, which includes 4 conditions $|\uparrow\uparrow\rangle$, $|\downarrow\downarrow\rangle$, $|\uparrow\downarrow\rangle$, and $|\downarrow\uparrow\rangle$. Therefore the sum equals to 4, and we have

$$(\hat{\mathbf{q}}\times\mathbf{h}\cdot\mathbf{s})^2 = h^2\sin^2\theta \tag{3.30}$$

For $q > 2k_f$ the integral will become

$$I(q) = \frac{2V}{(2\pi)^3N}\int d^3h h^2\sin^2\theta = \frac{3}{k_f^3}\frac{1}{10}k_f^5\int_{-1}^{1} d\cos\theta(1-\cos^2\theta) = \frac{2}{5}k_f^2 \tag{3.31}$$

For $q \le 2k_f$, it will be a little bit messy to evaluate $I(q)$, I just leave it here and finish it later. Our response function can now be written as

$$\begin{aligned}\chi^{coll}(q,\omega) &= S_f(q)\frac{\frac{1}{b(q)-\omega}+\frac{1}{b(q)+\omega}}{1-\frac{1}{4}S_f(q)I(q)\left(\frac{\partial\tilde{V}}{\partial q}\right)^2\left(\frac{1}{b(q)-\omega}+\frac{1}{b(q)+\omega}\right)^2} \\ &= \frac{2S_f(q)b(q)(b^2(q)-\omega^2)}{(b^2(q)-\omega^2)^2 - S_f(q)I(q)\left(\frac{\partial\tilde{V}}{\partial q}\right)^2 b^2(q)}\end{aligned} \tag{3.32}$$

For $q > 2k_f$,

$$\chi^{coll}(q,\omega) = \frac{2b(q)(b^2(q)-\omega^2)}{(b^2(q)-\omega^2)^2 - \frac{2k_f^2}{5}\left(\frac{\partial\tilde{V}}{\partial q}\right)^2 b^2(q)} \tag{3.33}$$

We will get two equations by finding the divergent condition

$$b^2(q) - \omega^2 = \pm\frac{\sqrt{2}k_f}{\sqrt{5}}\frac{\partial\tilde{V}}{\partial q}b(q) \tag{3.34}$$

And we can get 4 solutions for $q > 2k_f$ which means $b(q) = q^2$

$$\omega_1 = \sqrt{q^4 + \frac{\sqrt{2}k_f}{\sqrt{5}}\left(\frac{\partial\tilde{V}}{\partial q}\right)q^2} \tag{3.35}$$

$$\omega_2 = \sqrt{q^4 - \frac{\sqrt{2}k_f}{\sqrt{5}}\left(\frac{\partial\tilde{V}}{\partial q}\right)q^2} \tag{3.36}$$

$$\omega_3 = -\sqrt{q^4 - \frac{\sqrt{2}k_f}{\sqrt{5}}\left(\frac{\partial\tilde{V}}{\partial q}\right)q^2} = -\omega_2 \tag{3.37}$$

$$\omega_4 = -\sqrt{q^4 + \frac{\sqrt{2}k_f}{\sqrt{5}}\left(\frac{\partial\tilde{V}}{\partial q}\right)q^2} = -\omega_1 \tag{3.38}$$

Then we can write our response function as

$$\chi^{coll}(q,\omega) = \frac{2b(q)(b^2(q)-\omega^2)}{(\omega-\omega_1)(\omega-\omega_2)(\omega+\omega_2)(\omega+\omega_1)} \tag{3.39}$$

Then the imaginary part is

$$\operatorname{Im}\chi^{coll} = \pi\frac{2b(q)(b^2(q)-\omega^2)}{(\omega_1-\omega_2)(\omega+\omega_1)(\omega+\omega_2)}[\delta(\omega-\omega_1)-\delta(\omega-\omega_2)] \tag{3.40}$$

So the structure function is

$$\begin{aligned} S(q) = -\frac{1}{\pi}\int \operatorname{Im}\chi^{coll}(q,\omega) &= \frac{2b(q)(cb(q))}{(\omega_1-\omega_2)(\omega_1+\omega_2)2\omega_1} + \frac{2b(q)(cb(q))}{(\omega_1-\omega_2)(\omega_1+\omega_2)2\omega_2} \\ &= \frac{q^4\frac{2k_f}{\sqrt{10}}\frac{\partial\tilde{V}}{\partial q}}{2q^2\frac{2k_f}{\sqrt{10}}\frac{\partial\tilde{V}}{\partial q}\times\sqrt{q^4+\frac{\sqrt{2}k_f^2}{\sqrt{5}}\left(\frac{\partial\tilde{V}}{\partial q}\right)q^2}} + \frac{q^4\frac{2k_f}{\sqrt{10}}\frac{\partial\tilde{V}}{\partial q}}{2q^2\frac{2k_f}{\sqrt{10}}\frac{\partial\tilde{V}}{\partial q}\times\sqrt{q^4-\frac{\sqrt{2}k_f^2}{\sqrt{5}}\left(\frac{\partial\tilde{V}}{\partial q}\right)q^2}} \\ &= \frac{1}{2\sqrt{1+\frac{\sqrt{2}k_f}{\sqrt{5}q^2}\left(\frac{\partial\tilde{V}}{\partial q}\right)}} + \frac{1}{2\sqrt{1-\frac{\sqrt{2}k_f}{\sqrt{5}q^2}\left(\frac{\partial\tilde{V}}{\partial q}\right)}} \end{aligned} \tag{3.41}$$

Here $c = \frac{\sqrt{2}k_f}{\sqrt{5}}\frac{\partial\tilde{V}}{\partial q}$. Following similar steps, we can find the general form of the imaginary part of our response function is

$$\operatorname{Im}\chi^{coll} = \pi\frac{2S_f(q)b(q)(b^2(q)-\omega^2)}{(\omega_1-\omega_2)(\omega+\omega_1)(\omega+\omega_2)}[\delta(\omega-\omega_1)-\delta(\omega-\omega_2)] \tag{3.42}$$

While following equation

$$b^2(q) - \omega^2 = \pm c(q)b(q) \tag{3.43}$$

where $c(q) = \sqrt{S_f(q)I(q)}\frac{\partial \tilde{V}}{\partial q}$, we get

$$\omega_1 = \sqrt{b^2(q) + c(q)b(q)} \tag{3.44}$$

$$\omega_2 = \sqrt{b^2(q) - c(q)b(q)} \tag{3.45}$$

$$\omega_3 = -\sqrt{b^2(q) - c(q)b(q)} = -\omega_2 \tag{3.46}$$

$$\omega_4 = -\sqrt{b^2(q) + c(q)b(q)} = -\omega_1 \tag{3.47}$$

And the general form of structure function is

$$S(q) = -\frac{1}{\pi}\int \operatorname{Im}\chi^{coll} d\omega = \frac{2q^2 c(q)b(q)}{(\omega_1 - \omega_2)(\omega_1 + \omega_2)}\left(\frac{1}{\omega_1} + \frac{1}{\omega_2}\right) = \frac{q^2}{2}\left(\frac{1}{\omega_1} + \frac{1}{\omega_2}\right) \tag{3.48}$$

All we need to do is to evalua $b(q)$ and $c(q)$. We have already known that for $q \leq 2k_f$,

$$S_f(q) = \frac{3}{4k_f^3}\left(k_f^2 q - \frac{q^3}{12}\right) \tag{3.49}$$

So we have

$$b(q) = \frac{q^2}{S_f(q)} = \frac{4k_f^3 q}{3\left(k_f^2 - \frac{q^2}{12}\right)} \tag{3.50}$$

To evaluate $c(q)$, we need to evaluate $I(q)$ for $q \leq 2k_f$.

$$\begin{aligned}
I(q) &= \frac{2V}{(2\pi)^3 N}\int d^3h h^2 \sin^2\theta \\
&= \frac{2V}{(2\pi)^3 N}\left(\int_0^{2\pi} d\phi \int_{-q/2}^{k_f} dz \int_0^{\sqrt{k_f^2 - z^2}} d\rho\rho^3 - \int_0^{2\pi} d\phi \int_{-q/2}^{k_f - q} dz \int_0^{\sqrt{k_f^2-(z+q)^2}} d\rho\rho^3\right) \\
&= \frac{3}{8k_f^3}\left(\int_{-q/2}^{k_f} dz(k_f^2 - z^2)^2 - \int_{q/2}^{k_f} dz(k_f^2 - z^2)^2\right) \\
&= \frac{3}{8k_f^3}\left(k_f^5 + \frac{k_f^4 q}{2} - \frac{2}{3}k_f^5 - \frac{1}{12}k_f^2 q^3 + \frac{1}{5}k_f^5\right. \\
&\left. + \frac{1}{160}q^5 - k_f^5 + \frac{k_f^4 q}{2} + \frac{2}{3}k_f^5 - \frac{1}{12}k_f^2 q^3 - \frac{1}{5}k_f^5 + \frac{1}{160}q^5\right) \\
&= \frac{3}{8k_f^3}\left(k_f^4 q - \frac{k_f^2 q^3}{6} + \frac{q^5}{80}\right)
\end{aligned} \tag{3.51}$$

Therefore, our structure function for $q \leq 2k_f$ is

$$S(q) = \frac{q^2}{\sqrt{\frac{16k_f^6q^2}{9\left(k_f^2 - \frac{q^2}{12}\right)^2} + \frac{3q^2}{4\sqrt{2}k_f^3}\sqrt{\left(k_f^6q^2 - \frac{k_f^4q^4}{4} + \frac{19k_f^2q^6}{720} - \frac{q^8}{960}\right)}\left(\frac{\partial \tilde{V}}{\partial q}\right)}} + \frac{q^2}{\sqrt{\frac{16k_f^6q^2}{9\left(k_f^2 - \frac{q^2}{12}\right)^2} - \frac{3q^2}{4\sqrt{2}k_f^3}\sqrt{\left(k_f^6q^2 - \frac{k_f^4q^4}{4} + \frac{19k_f^2q^6}{720} - \frac{q^8}{960}\right)}\left(\frac{\partial \tilde{V}}{\partial q}\right)}} \tag{3.52}$$

We should notice here that the second term will not exist if its denominator is not real.

3.3 Derivation Including a Central Potential

In general, our interaction should contain a central interaction term, thus the general form of our interaction is

$$V_{int} = V_c(r_{12}) + V_{LS}(r_{12})\mathbf{L}\cdot\mathbf{S} \tag{3.53}$$

For such a central interaction we have already calculated that

$$\langle ph' | V_c(r_{12}) | hp' \rangle = \frac{\delta(\mathbf{q}-\mathbf{q}')}{N}\tilde{V}_c(q) \tag{3.54}$$

$$\langle pp' | V_c(r_{12}) | hh' \rangle = \frac{\delta(\mathbf{q}+\mathbf{q}')}{N}\tilde{V}_c(q) \tag{3.55}$$

The TDHF equations can now be written as

$$(\varepsilon_p - \varepsilon_h - \omega)x_{ph} + \frac{1}{N}\sum_{p'h'}\left[\delta(\mathbf{q}-\mathbf{q}')\left(\frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times(\mathbf{h}-\mathbf{h}') + \tilde{V}_c\right)x_{p'h'} + \delta(\mathbf{q}+\mathbf{q}')\left(\frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times(\mathbf{h}-\mathbf{h}') + \tilde{V}_c\right)y_{p'h'}\right] + \delta\tilde{H}(q) = 0 \tag{3.56}$$

$$(\varepsilon_p - \varepsilon_h + \omega)y_{ph} + \frac{1}{N}\sum_{p'h'}\left[\delta(\mathbf{q}+\mathbf{q}')\left(\frac{-i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times(\mathbf{h}-\mathbf{h}') + \tilde{V}_c\right)x_{p'h'} + \delta(\mathbf{q}-\mathbf{q}')\left(\frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times(\mathbf{h}-\mathbf{h}') + \tilde{V}_c\right)y_{p'h'}\right] + \delta\tilde{H}(q) = 0 \tag{3.57}$$

Using the same method, we will get 4 equations

$$\tilde{x}(q) = -\frac{1}{N}\sum_h \frac{1}{\varepsilon_p - \varepsilon_h - \omega}\left[\left(\frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times\mathbf{h} + \tilde{V}_c\right)(\tilde{x}(q)+\tilde{y}(q)) - \frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}(\tilde{x}'(q)-\tilde{y}'(q)) + \delta\tilde{H}(q)\right] \tag{3.58}$$

$$\tilde{y}(q) = -\frac{1}{N}\sum_h \frac{1}{\varepsilon_p - \varepsilon_h + \omega}\left[\left(\frac{-i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times\mathbf{h} + \tilde{V}_c\right)(\tilde{x}(q)+\tilde{y}(q)) + \frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}(\tilde{x}'(q)-\tilde{y}'(q)) + \delta\tilde{H}(q)\right] \tag{3.59}$$

$$\tilde{x}'(q) = -\frac{1}{N}\sum_h \frac{\hat{\mathbf{q}}\times\mathbf{h}}{\varepsilon_p - \varepsilon_h - \omega}\left[\left(\frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times\mathbf{h} + \tilde{V}_c\right)(\tilde{x}(q)+\tilde{y}(q)) - \frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}(\tilde{x}'(q)-\tilde{y}'(q)) + \delta\tilde{H}(q)\right] \tag{3.60}$$

$$\tilde{y}'(q) = -\frac{1}{N}\sum_h \frac{\hat{\mathbf{q}}\times\mathbf{h}}{\varepsilon_p - \varepsilon_h + \omega}\left[\left(\frac{-i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}}\times\mathbf{h} + \tilde{V}_c\right)(\tilde{x}(q)+\tilde{y}(q)) + \frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}(\tilde{x}'(q)-\tilde{y}'(q)) + \delta\tilde{H}(q)\right] \tag{3.61}$$

As we have proved previously

$$\sum_h \frac{\hat{\mathbf{q}}\times\mathbf{h}}{\varepsilon_p - \varepsilon_h \pm \omega} = 0 \tag{3.62}$$

We can exclude all 1st-order term of $\hat{\mathbf{q}}\times\mathbf{h}$, and get two equations

$$\begin{aligned}\tilde{x}(q)+\tilde{y}(q) = &-\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)[\tilde{V}_c(\tilde{x}(q)+\tilde{y}(q))+\delta\tilde{H}(q)]\\ &+\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\left[\frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}(\tilde{x}'(q)-\tilde{y}'(q))\right]\end{aligned} \tag{3.63}$$

$$\tilde{x}'(q)-\tilde{y}'(q) = -\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\left[\frac{i}{2}\frac{\partial \tilde{V}_{LS}}{\partial q}(\hat{\mathbf{q}}\times\mathbf{h})^2(\tilde{x}(q)+\tilde{y}(q))\right] \tag{3.64}$$

Combine these two equations we get

$$\left[1+\tilde{V}_c\chi_0 - \frac{1}{4N^2}\left(\frac{\partial \tilde{V}_{LS}}{\partial q}\right)^2\sum_h u(h,\omega)\sum_h(\hat{\mathbf{q}}\times\mathbf{h})^2u(h,\omega)\right](\tilde{x}(q)+\tilde{y}(q)) = \chi_0\delta\tilde{H}(q) \tag{3.65}$$

Therefore the general response function is, including the spin part

$$\chi(q,\omega) = \frac{\chi_0}{1+\tilde{V}_c\chi_0-\frac{1}{16N^2}\left(\frac{\partial \tilde{V}_{LS}}{\partial q}\right)^2\sum\limits_h u(h,\omega)\sum\limits_h(\hat{\mathbf{q}}\times\mathbf{h})^2u(h,\omega)} \tag{3.66}$$

This expression is exactly the same as our expectation. Following the same procedure, the expression of collective-mode response function is

$$\chi^{coll}(q,\omega) = \frac{2q^2(b^2(q)-\omega^2)}{(b^2(q)-\omega^2)^2 + 2q^2\tilde{V}_c(q)(b^2(q)-\omega^2) - c^2(q)b^2(q)} \tag{3.67}$$

here $b(q)$, $c(q)$ are the same as our previous derivation. To get all divergent conditions, we need to solve the equation

$$(b^2(q)-\omega^2)^2 + 2q^2\tilde{V}_c(q)(b^2(q)-\omega^2) - c^2(q)b^2(q) = 0 \tag{3.68}$$

This can be written as

$$b^2(q) - \omega^2 + q^2\tilde{V}_c(q) = \pm\sqrt{q^4\tilde{V}_c^2(q) + c^2(q)b^2(q)} \tag{3.69}$$

And we will get 4 solutions

$$\omega_1 = \sqrt{b^2(q) + q^2\tilde{V}_c(q) + \sqrt{q^4\tilde{V}_c^2(q) + c^2(q)b^2(q)}} \tag{3.70}$$

$$\omega_2 = \sqrt{b^2(q) + q^2\tilde{V}_c(q) - \sqrt{q^4\tilde{V}_c^2(q) + c^2(q)b^2(q)}} \tag{3.71}$$

$$\omega_3 = -\sqrt{b^2(q) + q^2\tilde{V}_c(q) - \sqrt{q^4\tilde{V}_c^2(q) + c^2(q)b^2(q)}} = -\omega_2 \tag{3.72}$$

$$\omega_4 = -\sqrt{b^2(q) + q^2\tilde{V}_c(q) + \sqrt{q^4\tilde{V}_c^2(q) + c^2(q)b^2(q)}} = -\omega_1 \tag{3.73}$$

The collective-mode response function can now be written as

$$\chi^{coll}(q,\omega) = \frac{2q^2(b^2(q)-\omega^2)}{(\omega-\omega_1)(\omega-\omega_2)(\omega+\omega_1)(\omega+\omega_2)} \tag{3.74}$$

The imaginary part is

$$\operatorname{Im}\chi^{coll}(q,\omega) = \pi\frac{2q^2(b^2(q)-\omega^2)}{(\omega_1-\omega_2)(\omega+\omega_1)(\omega+\omega_2)}[\delta(\omega-\omega_1) - \delta(\omega-\omega_2)] \tag{3.75}$$

Integrating over frequency over positve region, we get the structure function

$$\begin{aligned} S(q) = -\frac{1}{\pi}\int \operatorname{Im}\chi^{coll}(q,\omega) &= -\frac{2q^2(b^2(q)-\omega_1^2)}{(\omega_1-\omega_2)(2\omega_1)(\omega_1+\omega_2)} + \frac{2q^2(b^2(q)-\omega_2^2)}{(\omega_1-\omega_2)(2\omega_2)(\omega_1+\omega_2)} \\ &= \frac{q^2\left(q^2\tilde{V}_c(q) + \sqrt{q^4\tilde{V}_c^2(q) + c^2(q)b^2(q)}\right)}{2\sqrt{q^4\tilde{V}_c^2 + c^2(q)b^2(q)}}\left(\frac{1}{\omega_1} + \frac{1}{\omega_2}\right) \end{aligned} \tag{3.76}$$

Since the time is limited, we don't have time to check the correctness of this result. This will become our future work. On the other hand, we can see that even there are spin-dependency in our interaction and the Hartree-Fock state, our final result seems to be spin-independent. This result comes from the fact that the kinetic energy part and the spin part of our state are not correlated, and can be calculated separately. The effect of the sum of all the elements in the spin matrix turns out to be a constant factor, which doesn't play an important role. Our future work will focus on more complicated interaction in nuclear system, which would contain several terms with different dependencies. We will see if the spin dependency is important.

In Appendix B we attached an alternative, and more complete derivation of linear response function based on TDHF method, by showing all elements of the spin matrix $\boldsymbol{\sigma} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2$, and consider the spin-dependency of the density matrix.

Chapter 4

Central Potentail in One-dimensional Rashba Bosons

This chapter is the main work I have done during the Marshall program. A brife derivation of linear response theory using time-dependent Hartree-Fock(TDHF) method for 1D Rashba effect is introduced in this chapter. Instead of using the normal state, I calculated the ground states of 1D Rashba effect for one particle, and let our Hartree-Fock ground state as $2N$ particles in the Rashba ground states. Also, the collective-mode method and the numerical method are both used to calculate the static form factor.

4.1 Ground States of 1D Rashba Effect

The Hamiltonian of 1D Rashba Effect, for single particle, is

$$H_0 = \frac{\hat{p}_x^2}{2m} + \alpha\sigma_y\hat{p}_x + \Omega\sigma_z \tag{4.1}$$

where α is the strength of Rashba coupling, and Ω is the magnitude of the external constant field. We can see the spin operators σ_y and σ_z in our Hamiltonian, however, this Rashba effect is not a true spin effect. Instead, it is a pseudospin effect in cold atoms and the true dependence is in momentum. This dependence gives us an interesting case which has combined spin-momentum (or spin-orbit) states. The derivation for these states with a spin or orbital dependent interaction would be complicated. In this paper, we will study an interaction which depends only on coordinates space, to see if there are interesting results.

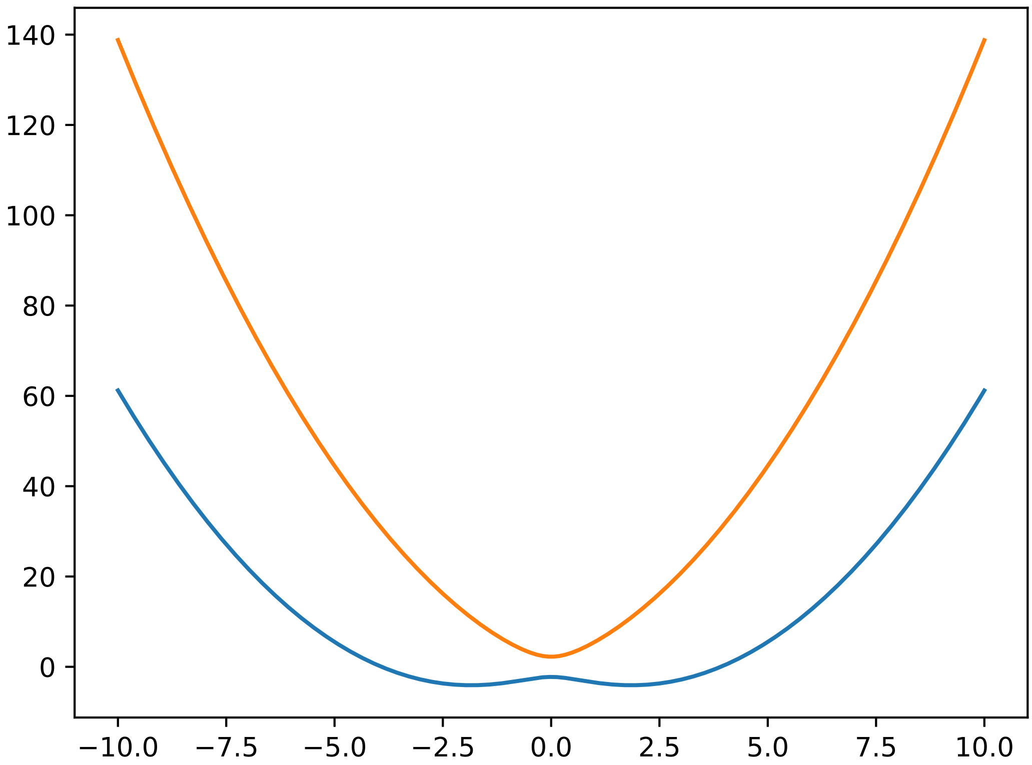

FIGURE 4.1: Qualitative plot of dispersion relations

From the Hamiltonian above, we can get 2 dispersion relations as FIG.4.1.

$$E^{\pm}(p_x) = \frac{p_x^2}{2m} \pm \sqrt{\Omega^2 + \alpha^2 p_x^2} \tag{4.2}$$

FIG.4.1 is just a qualitative plot of the dispersion relations. The actually shape of the dispersion relations, especially the lower curve, depends on the values of α and Ω. Here we will do a general derivation, and then talked about different conditions. The corresponding eigenstates for these two dispersion relations are

$$\left|\psi^{\pm}\right\rangle = \left|p_x, \xi^{\pm}_{p_x}\right\rangle = \left|p_x\right\rangle \left|\xi^{\pm}_{p_x}\right\rangle = \frac{\frac{1}{\sqrt{L}} e^{ip_x x}}{\sqrt{2(\Omega^2 + \alpha^2 p_x^2 \pm \Omega\sqrt{\Omega^2 + \alpha^2 p_x^2})}} \begin{pmatrix} \Omega \pm \sqrt{\Omega^2 + \alpha^2 p_x^2} \\ i\alpha p_x \end{pmatrix} \tag{4.3}$$

where L is the length of the system, which is to normalize the plane wave. An alternative form can be written as

$$\left|\psi^-\right\rangle = \left|p_x, \xi^-_{p_x}\right\rangle = \left|p_x\right\rangle \left|\xi^-_{p_x}\right\rangle = \frac{\frac{1}{\sqrt{L}}e^{ip_x x}}{\sqrt{2(\Omega^2 + \alpha^2 p_x^2 + \Omega\sqrt{\Omega^2 + \alpha^2 p_x^2})}} \begin{pmatrix} i\alpha p_x \\ \Omega \pm \sqrt{\Omega^2 + \alpha^2 p_x^2} \end{pmatrix} \tag{4.4}$$

$$\left|\psi^+\right\rangle = \left|p_x, \xi^+_{p_x}\right\rangle = \left|p_x\right\rangle \left|\xi^+_{p_x}\right\rangle = \frac{\frac{1}{\sqrt{L}}e^{ip_x x}}{\sqrt{2(\Omega^2 + \alpha^2 p_x^2 + \Omega\sqrt{\Omega^2 + \alpha^2 p_x^2})}} \begin{pmatrix} \Omega \pm \sqrt{\Omega^2 + \alpha^2 p_x^2} \\ i\alpha p_x \end{pmatrix} \tag{4.5}$$

The density of states $\rho = \frac{2N}{L}$ should be a constant for homogeneous systems. In our case we equally distributed $2N$ particles to 2 ground states, which is certainly a homogeneous system. For convenience, we may set $\rho = 1$, and all the derivations below are based on this.
From the dispersion relations above, we know the ground states should be in the lower one. To find the ground states we can minimize $E^-(p_x)$.

$$\frac{dE^-(p_x)}{dp_x} = \frac{p_x}{m} - \frac{\alpha^2 p_x}{\sqrt{\Omega^2 + \alpha^2 p_x^2}} = 0 \tag{4.6}$$

We can get the ground state momenta

$$h = \pm g = \begin{cases} \pm\frac{1}{\alpha}\sqrt{m^2\alpha^4 - \Omega^2}, & \alpha^4 > \Omega^2 \\ 0, & \alpha^4 \leq \Omega^2 \end{cases} \tag{4.7}$$

This is a general expression for the ground state momenta, even for the simple condition where $\alpha = 0$ or $\Omega = 0$. For simplicity we treat $\hbar = 1$ and $m = 1$. The product of these ground states are used as our Hartree-Fock state, to derive the TDHF equations and reformulate the linear response theory for a central potential, which will be shown in the next section. Now we should consider 3 simple cases.

- When both parameters are zeros, it reduced to the free particle expression and it is the simplest case which has been studied for a long time.

- For the condition where $\alpha = 0$ but $\Omega \neq 0$, it is just a vertical splitting of free-particle dispersion relation into 2 curves, which are shifts of the original curves by $\pm\Omega$. We can easily prove that the spin parts of the upper curve and the lower curve are always orthogonal, no matter what the value of p_x is. In this case all particles, as being bosons, will degenerate to the ground state, $g = 0$ of the lower curve. And the transition from the lower curve to the upper curve without spin flip is not allowed. Consider that the central potential contains no spin-flip part, which will result in transitions only within the lower curve. This has no difference with the free particle condition.

- The third condition is $\alpha \neq 0$ but $\Omega = 0$. This is a horizontal splitting of the free particle curve, which results in two ground state momenta $\pm g = \pm m\alpha$. The corresponding states of these two curves are

$$|p_x, \xi_{p_x}\rangle = \frac{\frac{1}{\sqrt{L}} e^{ip_x x}}{\sqrt{2}\alpha p_x} \begin{pmatrix} \alpha p_x \\ i\alpha p_x \end{pmatrix} \tag{4.8}$$

$$|p'_x, \xi_{p'_x}\rangle = \frac{\frac{1}{\sqrt{L}} e^{ip'_x x'}}{\sqrt{2}\alpha p'_x} \begin{pmatrix} i\alpha p'_x \\ \alpha p'_x \end{pmatrix} \tag{4.9}$$

If we just consider the spin parts and calculate the inner product, we get

$$\begin{pmatrix} \alpha p_x & -i\alpha p_x \end{pmatrix} \begin{pmatrix} i\alpha p'_x \\ \alpha p'_x \end{pmatrix} = i\alpha^2 p_x p'_x - i\alpha^2 p_x p'_x = 0 \tag{4.10}$$

This is valid for any values of p_x and p'_x. Therefore, the spin parts are orthogonal and the transition from one curve to the other is not permitted without spin flip. This is also the same as the free particle condition.

From the considerations above, it's not necessary to consider the case if $\alpha = 0$ or $\Omega = 0$, and all the derivations below are based on the difficult case when α and Ω are not zeros.

4.2 Reformulate Linear Response Theory

In this section, we reformulate linear response theory by time-dependent Hartree-Fock method. As we get the ground state of the Rashba bosons, we can now define our Hartree-Fock ground state as

$$|\Psi_0\rangle = \prod_{h=\pm g} (a^\dagger_{h\xi_h^-})^{N_h} |0\rangle \tag{4.11}$$

Here we have a restriction $N_g = N_{-g} = N$. It is the case when two ground states are equally occupied. Notice here that the Hartree-Fock state is the tensor product of all $2N$ ground states, and we have assumed that we can always generalize creation and annihilation operators which satisfy

$$a^\dagger_{p\xi_p} |0\rangle = |p, \xi_p\rangle \tag{4.12}$$

$$[a_{p\xi_p}, a^\dagger_{p'\xi'_p}] = \delta_{pp'} \delta_{\xi_p \xi_{p'}} \tag{4.13}$$

This assumption should be correct because our Schrödinger equation is linear. These operators satisfy the commutation relation because our system is bosonic system. We should keep in mind about this since now, because our previous derivation of TDHF equations are from a Fermi sea, which contains creation and annihilation operators satisfying the anti-commutation relation. Following the above expression of our Hartree-Fock ground state, which is a stationary state, we can generalize the form of time-dependent state, similar to what we did in the Fermi sea derivation, as

$$|\Psi(t)\rangle = e^{-iE_0t}\exp\left(\sum_{ph\xi_p} c_{ph\xi_p\xi_h^-}(t)a^\dagger_{p\xi_p}a_{h\xi_h^-}\right)|\Psi_0\rangle\,/\text{Norm} \tag{4.14}$$

Our total Hamiltonian is now

$$H = H_0 + V \tag{4.15}$$

where the second quantization form of our interaction is

$$V = \frac{1}{2}\sum_{\substack{\alpha\beta\gamma\delta\\ \xi_\alpha\xi_\beta\xi_\gamma\xi_\delta}} \langle\alpha\beta\xi_\alpha\xi_\beta|\,V\,|\gamma\delta\xi_\gamma\xi_\delta\rangle\, a^\dagger_{\alpha\xi_\alpha}a^\dagger_{\beta\xi_\beta}a_{\delta\xi_\delta}a_{\gamma\xi_\gamma} \tag{4.16}$$

Again we generalize a Lagrangian which is

$$\mathcal{L} = H - E_0 - V - i\frac{\partial}{\partial t} \tag{4.17}$$

where $E_0 = E_g$ is the ground state energy.
Now we can reformulate the TDHF equation following exactly the same way. However, there are some changes. The kinetic energy term for Fermi sea should change to H_0, which can be called "modified kinetic energy", because we have $\xi^\pm$ splitting. And we should calculated as

$$\begin{aligned}
&\langle\Psi(t)|\,(H_0 - E_0)\,|\Psi(t)\rangle\\
=&\sum_{\alpha\beta\xi_\alpha\xi_\beta}\langle\alpha\xi_\alpha|\,(H_0-E_0)\,|\beta\xi_\beta\rangle\,\langle\Psi_0|\,(1+\sum_{ph\xi_p}c^*_{ph\xi_p\xi_h^-}a^\dagger_{h\xi_h^-}a_{p\xi_p})a^\dagger_{\alpha\xi_\alpha}a_{\beta\xi_\beta}\\
&(1+\sum_{p'h'\xi_{p'}}c_{p'h'\xi_{p'}\xi_{h'}^-}a^\dagger_{p'\xi_{p'}}a_{h'\xi_{h'}})\,|\Psi_0\rangle\\
=&(E^\pm(p)-E^-(h))(1+|c_{ph}|^2)
\end{aligned} \tag{4.18}$$

Also, for the interaction part, we should rewrite to

$$\left\langle ph'\xi_p\xi_{h'}^-\right|V\left|hp'\xi_h^-\xi_{p'}\right\rangle = \left\langle ph'\right|V\left|hp'\right\rangle\left\langle\xi_p\xi_{h'}^-\middle|\xi_h^-\xi_{p'}\right\rangle = \frac{1}{2N}\tilde{V}(q)\delta(q-q')\left\langle\xi_p\xi_{h'}^-\middle|\xi_h^-\xi_{p'}\right\rangle \tag{4.19}$$

$$\left\langle pp'\xi_p\xi_{p'}\right|V\left|hp'\xi_h^-\xi_{h'}^-\right\rangle = \left\langle pp'\right|V\left|hh'\right\rangle\left\langle\xi_p\xi_{p'}\middle|\xi_h^-\xi_{h'}^-\right\rangle = \frac{1}{2N}\tilde{V}(q)\delta(q+q')\left\langle\xi_p\xi_{p'}\middle|\xi_h^-\xi_{h'}^-\right\rangle \tag{4.20}$$

Here we used again that $p = h + q$, $p' = h' + q'$. We should now compare the sum of these two expression. Since we have two "hole" states, for h' there are only two conditions $h' = \pm h$. We can get the two expressions

$$\sum_{\substack{p'=h'+q'\\h'=\pm h\\\xi_{p'}=\xi^{\pm}_{p'}}} \langle ph'\xi_p\xi^-_{h'}|\, V\, |hp'\xi^-_h\xi_{p'}\rangle = \frac{1}{2N}\tilde{V}(q) \sum_{\substack{p'=h'+q'\\h'=\pm h\\\xi_{p'}=\xi^{\pm}_{p'}}} \delta(q-q')\langle \xi_p|\xi^-_h\rangle \langle \xi^-_{h'}|\xi_{p'}\rangle$$
$$= \frac{1}{2N}\tilde{V}(q)\langle \xi_p|\xi^-_h\rangle \sum_{\xi=\xi^{\pm}} [\langle \xi^-_h|\xi_{h+q}\rangle + \langle \xi^-_{-h}|\xi_{-h+q}\rangle] \tag{4.21}$$

$$\sum_{\substack{p'=h'+q'\\h'=\pm h\\\xi_{p'}=\xi^{\pm}_{p'}}} \langle pp'\xi_p\xi_{p'}|\, V\, |hh'\xi^-_h\xi^-_{h'}\rangle = \frac{1}{2N}\tilde{V}(q) \sum_{\substack{p'=h'+q'\\h'=\pm h\\\xi_{p'}=\xi^{\pm}_{p'}}} \delta(q+q')\langle \xi_p|\xi^-_h\rangle \langle \xi_{p'}|\xi^-_{h'}\rangle$$
$$= \frac{1}{2N}\tilde{V}(q)\langle \xi_p|\xi^-_h\rangle \sum_{\xi=\xi^{\pm}} [\langle \xi_{h-q}|\xi^-_h\rangle + \langle \xi_{-h-q}|\xi^-_{-h}\rangle] \tag{4.22}$$

It's easy to verify that

$$\langle \xi^-_h|\xi_{h+q}\rangle = \langle \xi_{-h-q}|\xi^-_{-h}\rangle \tag{4.23}$$
$$\langle \xi^-_{-h}|\xi_{-h+q}\rangle = \langle \xi_{h-q}|\xi^-_h\rangle \tag{4.24}$$

Also remember that we have $|h| = |g|$. Therefore

$$\begin{aligned}\sum_{\substack{p'=h'+q'\\h'=\pm h\\\xi_{p'}=\xi^{\pm}_{p'}}} \langle ph'\xi_p\xi^-_{h'}|\, V\, |hp'\xi^-_h\xi_{p'}\rangle &= \sum_{\substack{p'=h'+q'\\h'=\pm h\\\xi_{p'}=\xi^{\pm}_{p'}}} \langle pp'\xi_p\xi_{p'}|\, V\, |hh'\xi^-_h\xi^-_{h'}\rangle \\ &= \frac{1}{2N}\tilde{V}(q)\langle \xi_p|\xi^-_h\rangle \sum_{\substack{h'=\pm g\\\xi=\xi^{\pm}}} \langle \xi^-_{h'}|\xi_{p'}\rangle\end{aligned} \tag{4.25}$$

The form of density is very similar to the normal state density

$$\begin{aligned}&\rho(t) = \langle\Psi(t)|\,\hat{\rho}\,|\Psi(t)\rangle = \\ &\sum_{\alpha\beta}\langle\alpha|\,\hat{\rho}\,|\beta\rangle\langle\Psi_0|\,(1+\sum_{ph\xi_p} c^*_{ph\xi_p\xi^-_h} a^\dagger_{h\xi^-_h} a_{p\xi_p})a^\dagger_{\alpha\xi\alpha}a_{\beta\xi_\beta}(1+\sum_{p'h'\xi_{p'}} c_{p'h'\xi_{p'}\xi^-_{h'}} a^\dagger_{p'\xi_{p'}} a_{h'\xi^-_{h'}})\,|\Psi_0\rangle \\ &= \mathrm{Tr}(\rho) + \delta\rho(t)\end{aligned} \tag{4.26}$$

The change of density $\delta\rho(t)$ is

$$\delta\rho(t) = \sum_{ph\xi_p}(c^*_{ph\xi_p\xi^-_h}\langle\xi_p|\xi^-_h\rangle\langle h|\,\hat{\rho}\,|p\rangle + c_{ph\xi_p}\langle\xi^-_h|\xi_p\rangle\langle p|\,\hat{\rho}\,|h\rangle) \tag{4.27}$$

Then we should consider the perturbation $\delta H(r)$, which is quite similar to the $\delta\rho(t)$

$$\begin{aligned} \left\langle h\xi_h^- \right| \delta H(r) \left| p\xi_p \right\rangle = \left\langle p\xi_p \right| \delta H(r) \left| h\xi_h^- \right\rangle = \left\langle p \right| \delta H(r) \left| h \right\rangle \left\langle \xi_p \middle| \xi_h^- \right\rangle \\ = \frac{1}{2N}\delta\tilde{H}(q) \left\langle \xi_p \middle| \xi_h^- \right\rangle = \delta\tilde{h}(q,\xi_q) = \delta\tilde{h}(q) \left\langle \xi_p \middle| \xi_h^- \right\rangle \end{aligned} \tag{4.28}$$

As we assume a real perturbation. Now if we use the harmonic expression $c(t) = xe^{-i\omega t} + ye^{i\omega t}$, the TDHF equations will become

$$(E^{\pm}(p) - E^{-}(h) - \omega)x_{ph\xi_p\xi_h^-} + \frac{1}{2N}\tilde{V}(q) \left\langle \xi_p \middle| \xi_h^- \right\rangle \sum_{\substack{h' \\ \xi=\xi^{\pm}}} \left\langle \xi_{h'}^- \middle| \xi_{p'} \right\rangle (x_{p'h'\xi_{p'}\xi_{h'}^-} + y_{p'h'\xi_{p'}\xi_{h'}^-})$$
$$+ \delta\tilde{h}(q,\xi_q) = 0 \tag{4.29}$$
$$(E^{\pm}(p) - E^{-}(h) + \omega)y_{ph\xi_p\xi_h^-} + \frac{1}{2N}\tilde{V}(q) \left\langle \xi_p \middle| \xi_h^- \right\rangle \sum_{\substack{h' \\ \xi=\xi^{\pm}}} \left\langle \xi_{h'}^- \middle| \xi_{p'} \right\rangle (x_{p'h'\xi_{p'}\xi_{h'}^-} + y_{p'h'\xi_{p'}\xi_{h'}^-})$$
$$+ \delta\tilde{h}(q,\xi_q) = 0 \tag{4.30}$$

Notice here that we have 4 equations, 2 for $\xi_p = \xi_p^+$ and $E(p) = E^+(p)$, 2 for $\xi_p = \xi_p^-$ and $E(p) = E^-(p)$. We can define

$$\tilde{x}(q,\xi_q) = \frac{1}{2N} \sum_{\substack{h' \\ \xi=\xi^{\pm}}} \left\langle \xi_{h'}^- \middle| \xi_{p'} \right\rangle x_{p'h'\xi_{p'}\xi_{h'}^-} \tag{4.31}$$

$$\tilde{y}(q,\xi_q) = \frac{1}{2N} \sum_{\substack{h' \\ \xi=\xi^{\pm}}} \left\langle \xi_{h'}^- \middle| \xi_{p'} \right\rangle y_{p'h'\xi_{p'}\xi_{h'}^-} \tag{4.32}$$

Then the two equations can be rewritten to

$$\tilde{x}(q,\xi_q) = -\frac{1}{2N} \sum_{\substack{h \\ \xi=\xi^{\pm}}} \frac{\left\langle \xi_h^- \middle| \xi_p \right\rangle}{E^{\pm}(p) - E^{-}(h) - \omega} \left[\tilde{V}(q) \left\langle \xi_p \middle| \xi_h^- \right\rangle (\tilde{x}(q,\xi_q) + \tilde{y}(q,\xi_q)) + \delta\tilde{h}(q,\xi_q)\right] \tag{4.33}$$

$$\tilde{y}(q,\xi_q) = -\frac{1}{2N} \sum_{\substack{h \\ \xi=\xi^{\pm}}} \frac{\left\langle \xi_h^- \middle| \xi_p \right\rangle}{E^{\pm}(p) - E^{-}(h) + \omega} \left[\tilde{V}(q) \left\langle \xi_p \middle| \xi_h^- \right\rangle (\tilde{x}(q,\xi_q) + \tilde{y}(q,\xi_q)) + \delta\tilde{h}(q,\xi_q)\right] \tag{4.34}$$

We will get

$$\tilde{x}(q,\xi_q) + \tilde{y}(q,\xi_q) = \frac{\chi_0'}{1 - \tilde{V}(q)\chi_0'}\delta\tilde{h}(q) \tag{4.35}$$

Here

$$\chi_0' = -\frac{1}{2N} \sum_{\substack{h \\ \xi=\xi^{\pm}}} |\left\langle \xi_h^- \middle| \xi_p \right\rangle|^2 \left(\frac{1}{E^{\pm}(p) - E^{-}(h) - \omega} + \frac{1}{E^{\pm}(p) - E^{-}(h) + \omega}\right) \tag{4.36}$$

is the non-interacting response function. An alternative form is to change $\sum_{h'}$ to $N\sum_{h'=\pm g}$, since there is N-degeneracy for each ground state. And we can write χ_0' as

$$\chi_0' = -\sum_{\substack{h=\pm g\\ \xi=\xi^\pm}} \frac{1}{2}|\left\langle \xi_h^- \middle| \xi_p \right\rangle|^2 \left(\frac{1}{E^\pm(p) - E^-(h) - \omega} + \frac{1}{E^\pm(p) - E^-(h) + \omega} \right) \tag{4.37}$$

This form is useful in numerical calculation, which will be done later. Our response function is

$$\chi(q,\omega) = \frac{\chi_0'}{1 - \tilde{V}(q)\chi_0'} \tag{4.38}$$

This expression is quite similar, but not exactly the same as our original response function for normal state. The difference comes from the non-orthogonal spin part, even though the total eigenvectors are orthogonal.

4.3 Collective Approximation

The "collective approximation" is implicit to the Jastrow-Feenberg or fixed node approximation. Being aware of where the approximation comes from, it is easy to relax if appropriate.

Now we should consider the collective mode approximation. The dynamic form factor for non-interacting 1D Rashba system should have the form

$$S_F(q,\omega) = \frac{1}{2N} \sum_{\substack{h\\ \xi=\xi^\pm}} |\rho_{q\xi_q}|^2 \delta(\omega - \omega_{q\xi_q}) \tag{4.39}$$

Here

$$\rho_{q\xi_q} = \left\langle \xi_h^- \middle| \xi_{h+q} \right\rangle \tag{4.40}$$

$$\omega_{q\xi_q} = \omega_{h+q,\xi_{h+q}} - \omega_{h,\xi_h^-} \tag{4.41}$$

Integrate over frequency we get the static form factor

$$S_F(q) = \int_0^\infty d\omega S_F(q,\omega) = \sum_{\substack{h\\ \xi=\xi^\pm}} |\rho_{q\xi_q}|^2 = \frac{1}{2N}\sum_h \sum_{\xi=\xi^\pm} \left\langle \xi_h^- \middle| \xi_{h+q} \right\rangle \left\langle \xi_{h+q} \middle| \xi_h^- \right\rangle = \frac{1}{2N}\sum_h = 1 \tag{4.42}$$

Notice here that we have $2N$ particles equally distributed in the 2 ground states, so the sum $\sum_h = 2N$. It is not surprising to get the static form facor as 1, since we are studying a bosonic system. Using the f-sum rules, it's easy to get the collective form of non-interacting response function as

$$\chi_0^{\text{coll}} = -\frac{1}{\omega_F(q) - \omega} - \frac{1}{\omega_F(q) + \omega} = -\frac{2\omega_F(q)}{(\omega_F(q))^2 - \omega^2} \tag{4.43}$$

here $\omega_F(q) = q^2/2m$ is the energy of a free particle. We see that this collective form is the same as the one of the normal Bose system. The collective form of interacting response function is now

$$\chi^{\text{coll}}(q,\omega) = \frac{\chi_0^{\text{coll}}(q,\omega)}{1 - \tilde{V}(q)\chi_0^{\text{coll}}(q,\omega)} = \frac{2\omega_F(q)}{\omega_F^2 - \omega^2 + 2\tilde{V}(q)\omega_F(q)} = \frac{2\omega_F(q)}{(\omega + \omega^{coll}(q))(\omega - \omega^{coll}(q))} \tag{4.44}$$

Here

$$\omega^{coll}(q) = \sqrt{\omega_F^2(q) + 2\tilde{V}(q)\omega_F(q)} = \sqrt{\frac{q^4}{4m^2} + \frac{\tilde{V}(q)q^2}{m}} \tag{4.45}$$

which is just the Bogoliubov energy.

We should choose a complex frequency by changing $\omega \to \omega - i\eta$, we will get the imaginary part of the response function for the limit $\eta \to 0$ that

$$\text{Im}\Big\{\chi^{coll}(q,\omega)\Big\} = -\pi\frac{2\omega_F(q)}{\omega + \omega^{coll}(q)}\delta(\omega - \omega^{coll}(q)) \tag{4.46}$$

Then the static form factor of the interacting system is

$$S^{\text{coll}}(q) = -\frac{1}{\pi}\int_0^\infty d\omega\,\text{Im}\Big\{\chi^{coll}(q,\omega)\Big\} = \frac{\omega_F(q)}{\omega^{coll}(q)} = \frac{q^2}{\sqrt{q^4 + 4m\tilde{V}(q)q^2}} \tag{4.47}$$

Going beyond the collective approximation we recall that the system exact free response function has the form

$$\chi_0(q,\omega) = \sum_{i=1}^{4} p_i \frac{2\omega_{0i}}{(\omega + I\eta)^2 - \omega_{0i}^2} \tag{4.48}$$

with

$$\sum_{i=1}^{4} p_i = 1$$

The RPA response function is then the a superposition of three or four discrete modes, which can be found by solving the equation

$$1 - \tilde{V}(q)\chi_0(q,\omega_j) = 0 \tag{4.49}$$

This equation is in principle solvable analytically, however, the expressions for the solutions are too complicated to be used. It is much simpler to solve the equation numerically by a Newton procedure.

For the purpose of solving the local parquet equations, we can take a look at our response function, its expression can be written in a series form

$$\begin{aligned}\chi(q,\omega) &= \chi_0(q,\omega)+\chi_0(q,\omega)\tilde{V}(q)\chi_0(q,\omega)\\ &\quad+\chi_0(q,\omega)\tilde{V}(q)\chi_0(q,\omega)\tilde{V}(q)\chi_0(q,\omega)+\dots\\ &\equiv \chi_0(q,\omega)+\chi_0(q,\omega)W(q,\omega)\chi_0(q,\omega) \qquad (4.50)\end{aligned}$$

where

$$W(q,\omega)=\frac{\tilde{V}(q)}{1-\tilde{V}(q)\chi_0(q,\omega)} \qquad (4.51)$$

The localization procedure of the parquet-diagram summation defines now an energy independent induced interaction $w_I(q)$ which can be written as $w_I(q)=W(q,\bar{\omega}(q))$, where $\bar{\omega}(q)$ is an average frequency determined such that

$$\begin{aligned}S(q) &= -\operatorname{Im}\int_0^\infty \frac{d\omega}{\pi}\left[\chi_0(q,\omega)+\chi_0(q,\omega)W(q,\omega)\chi_0(q,\omega)\right]\\ &= -\operatorname{Im}\int_0^\infty \frac{d\omega}{\pi}\left[\chi_0(q,\omega)+\chi_0(q,\omega)W(q,\bar{\omega}(q))\chi_0(q,\omega)\right] \qquad (4.52)\end{aligned}$$

This can now be evaluated in different ways:

- In the collective approximation the first term is 1, and the second term is

$$-W(q,\bar{\omega}(q))\operatorname{Im}\int_0^\infty \frac{d\omega}{\pi}\chi_0^2(q,\omega)=-W(q,\bar{\omega})/\omega_F(q) \qquad (4.53)$$

  Hence,

$$w_I(q,\omega)\equiv W(q,\bar{\omega})=-\omega_F(q)(S^{\rm coll}(q)-1) \qquad (4.54)$$

  We can also calculate $\bar{\omega}(q)$ but we do not need to for the time being.

- Avoiding the collective approximation, we get instead

$$\operatorname{Im}\int_0^\infty \frac{d\omega}{\pi}\chi_0^2(q,\omega)=\sum_{i,j}\frac{2p_ip_j}{\omega_{0i}+\omega_{0j}} \qquad (4.55)$$

  and, hence,

$$w_I(q,\omega)\equiv W(q,\bar{\omega})=-\frac{S(q)-1}{\sum_{i,j}\frac{2p_ip_j}{\omega_{0i}+\omega_{0j}}} \qquad (4.56)$$

  which needs to be examined if it is good or not.

4.4 Find Poles of the Response Function

In this section we are trying to find poles of the response function, which is to solve

$$1 - \tilde{V}(q)\chi_0' = 0 \tag{4.57}$$

numerically, as we have argue that the analytical solutions of this formula are too complicated to use. Now we should transform this expression into polynomial form. We now put the expression to of χ_0' to the equation, and get

$$1 + \tilde{V}(q)\sum_{n}^{4} p_n \frac{2\omega_n}{\omega_n^2 - \omega^2} = 0 \tag{4.58}$$

Here $p_n = \frac{1}{2}|\rho_n|^2$ is the probability of transition from ground state to n state. For convenience, we type out the full expressions of all ω_ns and p_ns, as we set $m = 1$,

$$\omega_1 = \frac{(g+q)^2}{2} - \sqrt{\Omega^2 + \alpha^2(g+q)^2} - \frac{g^2}{2} + \sqrt{\Omega^2 + \alpha^2 g^2} \tag{4.59}$$

$$\omega_2 = \frac{(g+q)^2}{2} + \sqrt{\Omega^2 + \alpha^2(g+q)^2} - \frac{g^2}{2} + \sqrt{\Omega^2 + \alpha^2 g^2} \tag{4.60}$$

$$\omega_3 = \frac{(g-q)^2}{2} - \sqrt{\Omega^2 + \alpha^2(g-q)^2} - \frac{g^2}{2} + \sqrt{\Omega^2 + \alpha^2 g^2} \tag{4.61}$$

$$\omega_4 = \frac{(g-q)^2}{2} + \sqrt{\Omega^2 + \alpha^2(g-q)^2} - \frac{g^2}{2} + \sqrt{\Omega^2 + \alpha^2 g^2} \tag{4.62}$$

$$p_1 = \frac{[\alpha^2 g(g+q) + (\Omega + \sqrt{\Omega^2 + \alpha^2(g+q)^2})(\Omega + \sqrt{\Omega^2 + \alpha^2 g^2})]^2}{8(\alpha^2(g+q)^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2(g+q)^2})(\alpha^2 g^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2 g^2})} \tag{4.63}$$

$$p_2 = \frac{[\alpha g(\Omega + \sqrt{\Omega^2 + \alpha^2(g+q)^2}) + \alpha(g+q)(\Omega + \sqrt{\Omega^2 + \alpha^2 g^2})]^2}{8(\alpha^2(g+q)^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2(g+q)^2})(\alpha^2 g^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2 g^2})} \tag{4.64}$$

$$p_3 = \frac{[\alpha^2 g(g-q) + (\Omega + \sqrt{\Omega^2 + \alpha^2(g-q)^2})(\Omega + \sqrt{\Omega^2 + \alpha^2 g^2})]^2}{8(\alpha^2(g-q)^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2(g-q)^2})(\alpha^2 g^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2 g^2})} \tag{4.65}$$

$$p_4 = \frac{[\alpha(-g)(\Omega + \sqrt{\Omega^2 + \alpha^2(q-g)^2}) - \alpha(q-g)(\Omega + \sqrt{\Omega^2 + \alpha^2 g^2})]^2}{8(\alpha^2(q-g)^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2(q-g)^2})(\alpha^2 g^2 + \Omega^2 + \Omega\sqrt{\Omega^2 + \alpha^2 g^2})} \tag{4.66}$$

Now we can write a simple rtsafe algorithm to find all the poles of the response function, and then calculate the static form factor using theorem of residue. FIG.4.2 shows the static form factor calculated by collective-mode approximation and numerical methods. The one calculated by the collective-mode approximation is just the Bogoliubov formula, which is the "Bogoliubov" curve in the figure. We can see a sharp valley in the numerical result, which is when $q = 2 * g$, where zero-energy transition,from ground state $-g$ to ground state g happens. Also, we can see that these two curves don't agree. As we believe that the numerical result is more accurate, the Bogoliubov formula does not work in our case. As we can see in the non-interacting response function, the probability of transition is the inner product of the spin parts, which means the spin-dependency

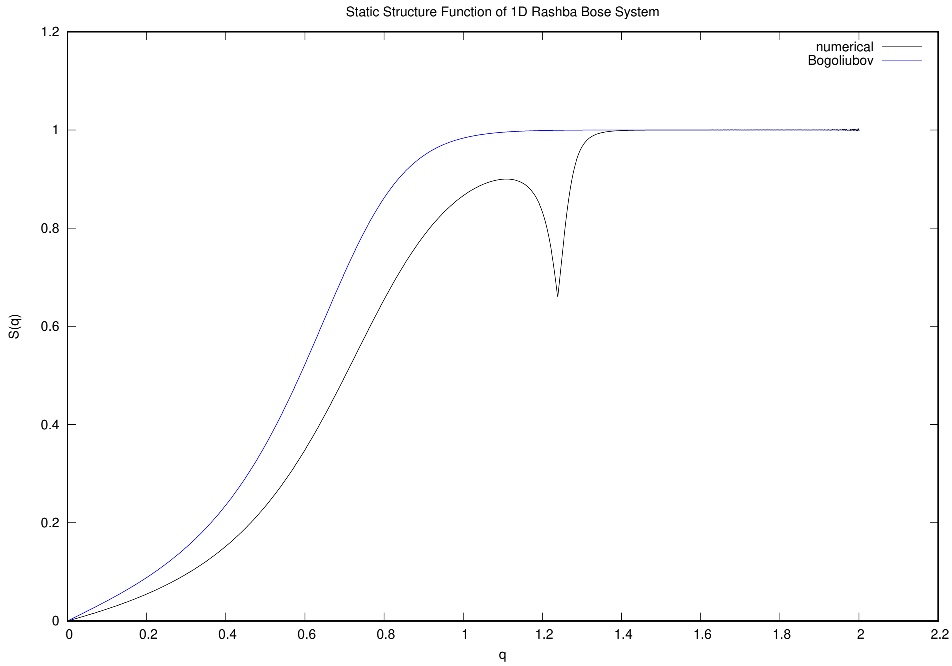

FIGURE 4.2: Qualitative plot of dispersion relations

plays an important role, even we are not considering a spin-dependent interaction. This unusual phenomenon happens only in systems of this kind, where the spin part of the eigenstate is a function of momentum, which means the kinetic energy part and the spin part of the eigenstate are correlated. It would be an interesting study if we consider an spin-dependent interaction. This will be done in the future.

Appendix A

A trial to work out the full expression of spin-orbit response function

The other way to calculate the static structure function $S(q)$ is to figure out the last term of the denominator $\chi^{(2)}$, and then calculate numerically. Here we can prove that it is impossible to evaluate the analytical expression of $S(q)$ because the analytical expression of our response function is too complicated. The spin part is not outside the integral, so we can use a trick to calculate the orbital part by choosing $\hat{\mathbf{q}}$ in z-direction. Then we can use the formula

$$(\hat{\mathbf{q}} \times \mathbf{h} \cdot \mathbf{s})^2 = h^2 \sin^2 \theta \tag{A.1}$$

which has been proved previously. And we can turn the $\chi_1^{(2)}$ into integral form as

$$\begin{aligned} \chi_1^{(2)} = \frac{1}{N} \sum_h (\hat{\mathbf{q}} \times \mathbf{h} \cdot \mathbf{s})^2 v(h, \omega) = \nu \int \frac{d^3 h}{(2\pi)^3 \rho_0} n(h)(1 - n(\mathbf{h} + \mathbf{q})) \\ \times \left[\frac{h^2 \sin^2 \theta}{\frac{\hbar^2}{2m}[q^2 + 2qz] - \omega} - \frac{h^2 \sin^2 \theta}{\frac{\hbar^2}{2m}[q^2 + 2qz] + \omega} \right] \end{aligned} \tag{A.2}$$

For this integral we always have a restriction that $|\mathbf{h}+\mathbf{q}| > 1$, as we chose all momenta measured in units of k_F, and all energies in units of the Fermi energy for simplicity. Now consider the simplest case that $q > 2$ so the restriction is always satisfied. We can rewrite our integral into cylindrical coordinates form.

$$\frac{3}{4\pi} \int_{-1}^{1} dz \int_0^{\sqrt{1-z^2}} d\rho \int_0^{2\pi} d\phi \rho \left[\frac{\rho^2}{q^2 + 2qz - \omega} - \frac{\rho^2}{q^2 + 2qz + \omega} \right] \tag{A.3}$$

We can then just look closer to the first term in the integral, since the two terms are quite similar. The integral of the first term is

$$\begin{aligned} I_1 &= \int_{-1}^{1} dz \int_0^{\sqrt{1-z^2}} d\rho \int_0^{2\pi} d\phi \frac{\rho^3}{q^2+2qz-\omega} \\ &= \int_{-1}^{1} dz \frac{\frac{1}{2}\pi(1-z^2)^2}{q^2+2qz-\omega} \\ &= \int_{-1}^{1} dz \frac{\frac{1}{2}\pi(1-2z^2+z^4)}{q^2+2qz-\omega} \end{aligned} \tag{A.4}$$

Use the integrals

$$\int \frac{ax^2}{bx+c}dx = \frac{ac^2\log(bx+c)}{b^3} + \frac{ax(bx-2c)}{2b^2} \tag{A.5}$$

$$\int \frac{ax^4}{bx+c}dx = a\left(\frac{c^4\log(bx+c)}{b^5} - \frac{c^3x}{b^4} + \frac{c^2x^2}{2b^3} - \frac{cx^3}{3b^2} + \frac{x^4}{4b}\right) \tag{A.6}$$

The integral of the first term then become

$$\begin{aligned} I_1 &= \frac{1}{4q}\pi\left(\log\left(\frac{q^2+2q-\omega}{q^2-2q-\omega}\right) - \frac{1}{2q^2}(q^2-\omega)^2\log\left(\frac{q^2+2q-\omega}{q^2-2q-\omega}\right) + \frac{2}{q}(q^2-\omega)\right. \\ &\qquad \left. + \frac{1}{16q^4}(q^2-\omega)^4\log\left(\frac{q^2+2q-\omega}{q^2-2q-\omega}\right) - \frac{(q^2-\omega)^3}{4q^3} - \frac{q^2-\omega}{3q}\right) \\ &= \frac{1}{4q}\pi\left[\left(1-\frac{1}{2q^2}(q^2-\omega)^2+\frac{1}{16q^4}(q^2-\omega)^4\right)\log\left(\frac{q^2+2q-\omega}{q^2-2q-\omega}\right) + \frac{(q^2-\omega)(17q^2+\omega)^2}{12q^3}\right] \\ &= \frac{1}{4q}\pi\left[\left(1-\frac{1}{4q^2}(q^2-\omega)^2\right)^2\log\left(\frac{q^2+2q-\omega}{q^2-2q-\omega}\right) + \frac{(q^2-\omega)(17q^2+\omega)^2}{12q^3}\right] \end{aligned} \tag{A.7}$$

Similarly, the integral of the second term is

$$\begin{aligned} I_2 &= \frac{1}{4q}\pi\left(\log\left(\frac{q^2+2q+\omega}{q^2-2q+\omega}\right) - \frac{1}{2q^2}(q^2+\omega)^2\log\left(\frac{q^2+2q+\omega}{q^2-2q+\omega}\right) + \frac{2}{q}(q^2+\omega)\right. \\ &\qquad \left. + \frac{1}{16q^4}(q^2+\omega)^4\log\left(\frac{q^2+2q+\omega}{q^2-2q+\omega}\right) - \frac{(q^2+\omega)^3}{4q^3} - \frac{q^2+\omega}{3q}\right) \\ &= \frac{1}{4q}\pi\left[\left(1-\frac{1}{2q^2}(q^2+\omega)^2+\frac{1}{16q^4}(q^2+\omega)^4\right)\log\left(\frac{q^2+2q+\omega}{q^2-2q+\omega}\right) + \frac{(q^2+\omega)(17q^2-\omega)^2}{12q^3}\right] \\ &= \frac{1}{4q}\pi\left[\left(1-\frac{1}{4q^2}(q^2+\omega)^2\right)^2\log\left(\frac{q^2+2q+\omega}{q^2-2q+\omega}\right) + \frac{(q^2+\omega)(17q^2-\omega)^2}{12q^3}\right] \end{aligned} \tag{A.8}$$

So we have

$$\chi_1^{(2)} = \frac{3}{4\pi}(I_1 - I_2) \tag{A.9}$$

This expression works only for the condition $q > 2k_f$. For the condtion $q \leq 2k_f$, we need to consider the integral region. The integral region for h should be inside a spher centered at the origin with radius 1, and outside the sphere centered at $-q$ on z-axis with radius 1. The integration region is shown in FIG.(A.1). The integral of the first term can now be written as

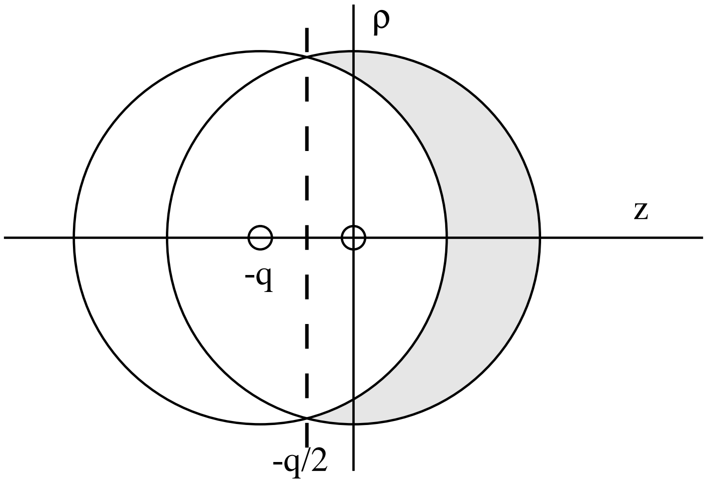

FIGURE A.1: The grey shaded area depicts the integration region.

$$
\begin{aligned}
I_3 &= \int_{-\frac{q}{2}}^{1} dz \int_0^{\sqrt{1-z^2}} d\rho \int_0^{2\pi} d\phi \frac{\rho^3 \cos^2 \phi s_{Ry}^2 + \rho^3 \sin^2 \phi s_{Rx}^2 - 2\rho^3 \sin\phi \cos\phi s_{Rx} s_{Ry}}{q^2 + 2qz - \omega} \\
&- \int_{-\frac{q}{2}}^{0} dz \int_0^{\sqrt{1-(z+q)^2}} d\rho \int_0^{2\pi} d\phi \frac{\rho^3 \cos^2 \phi s_{Ry}^2 + \rho^3 \sin^2 \phi s_{Rx}^2 - 2\rho^3 \sin\phi \cos\phi s_{Rx} s_{Ry}}{q^2 + 2qz - \omega} \\
&= \int_{-\frac{q}{2}}^{1} \frac{\frac{1}{2}\pi(1 - 2z^2 + z^4)}{q^2 + 2qz - \omega} dz - \int_{-\frac{q}{2}}^{0} \frac{\frac{1}{2}\pi(1 - 2(z+q)^2 + (z+q)^4)}{q^2 + 2qz - \omega} dz
\end{aligned}
\tag{A.10}
$$

The denominator of the second term can be rewritten as

$$
q^2 + 2qz - \omega = 2q(z+q) - q^2 - \omega \tag{A.11}
$$

Redefining $z + q \to z$, the integral is

$$
\begin{aligned}
I_3 &= \int_{-\frac{q}{2}}^{1} \frac{\frac{1}{2}\pi(1 - 2z^2 + z^4)}{q^2 + 2qz - \omega} dz - \int_{\frac{q}{2}}^{q} \frac{\frac{1}{2}\pi(1 - 2z^2 + z^4)}{2qz - q^2 - \omega} dz \\
&= \frac{1}{4q}\pi \left[\left(1 - \frac{(q^2-\omega)^2}{2q^2} + \frac{(q^2-\omega)^4}{16q^4} \right) \log\left(\frac{\omega - q^2 - 2q}{\omega} \right) - \frac{q - q^2 + \omega}{q} \right. \\
&- \frac{1}{4}(2\omega - 3q^2) - \frac{(q^2-\omega)^3(1+\frac{q}{2})}{8q^3} + \frac{(q^2-\omega)^2(1-\frac{q^2}{4})}{8q^2} - \frac{(q^2-\omega)(1+\frac{q^3}{8})}{6q} + \frac{1-\frac{q^4}{16}}{4} \\
&- \left(1 - \frac{(q^2+\omega)^2}{2q^2} + \frac{(q^2+\omega)^4}{16q^4} \right) \log\left(\frac{\omega - q^2}{\omega} \right) + \frac{5}{4}q^2 + \frac{1}{2}\omega \\
&\left. + \frac{(q^2+\omega)^3}{16q^2} + \frac{3(q^2+\omega)^2}{32} + \frac{7(q^2+\omega)q^2}{48} + \frac{15q^4}{64} \right]
\end{aligned}
\tag{A.12}
$$

Similarly,

$$\begin{aligned}
I_4 &= \int_{-\frac{q}{2}}^{1} \frac{\frac{1}{2}\pi(1-2z^2+z^4)}{q^2+2qz+\omega}dz - \int_{\frac{q}{2}}^{q} \frac{\frac{1}{2}\pi(1-2z^2+z^4)}{2qz-q^2+\omega}dz \\
&= \frac{1}{4q}\pi\left[\left(1-\frac{(q^2+\omega)^2}{2q^2}+\frac{(q^2+\omega)^4}{16q^4}\right)\log\left(\frac{\omega+q^2+2q}{\omega}\right)-\frac{q-q^2-\omega}{q}\right. \\
&+\frac{1}{4}(2\omega+3q^2)-\frac{(q^2+\omega)^3(1+\frac{q}{2})}{8q^3}+\frac{(q^2+\omega)^2(1-\frac{q^2}{4})}{8q^2}-\frac{(q^2+\omega)(1+\frac{q^3}{8})}{6q}+\frac{1-\frac{q^4}{16}}{4} \\
&-\left(1-\frac{(q^2-\omega)^2}{2q^2}+\frac{(q^2-\omega)^4}{16q^4}\right)\log\left(\frac{\omega+q^2}{\omega}\right)+\frac{5}{4}q^2-\frac{1}{2}\omega \\
&\left.+\frac{(q^2-\omega)^3}{16q^2}+\frac{3(q^2-\omega)^2}{32}+\frac{7(q^2-\omega)q^2}{48}+\frac{15q^4}{64}\right]
\end{aligned} \tag{A.13}$$

And we have, for $q \leq 2k_f$,

$$\chi_1^{(2)} = \frac{3}{4\pi}(I_3 - I_4) \tag{A.14}$$

As we can see, even we just consider the expression of $\chi_1^{(2)}$, it is a very complicated form. Therefore the full expression of χ should definitely be a complicated formula, which means we have no way to evaluate the analytical expression. Hence a numerical method should be used in the future, as we don't have enough time to finish this step during the exchange program.

Appendix B

An Alternative Derivation of Linear Response for Spin-Orbit Coupling

There is a huge mistake(or maybe we can call it huge approximation) in my previous derivations that I ignored the spin dependency of our density fluctuation $\delta\rho$. We can recall the formula of $\delta\rho(r,t)$ as

$$\delta\rho(r,t) = \sum_{ph\xi_p\xi_h} [c^*_{ph\xi_p\xi_h} \langle h\xi_h| \rho(r) |p\xi_p\rangle + c_{ph\xi_p\xi_h} \langle p\xi_p| \rho(r) |h\xi_h\rangle] \tag{B.1}$$

And I just assumed that $c_{ph\xi_p\xi_h}$ does not depend on the alignment of $\xi_p\xi_h$, which is not correct. It was not what I supposed to do but I just didn't look at it carefully. Also, the formula of the perturbation should be

$$\begin{aligned} \delta H(r,t) &= \sum_{ph\xi_p\xi_h} [c^*_{ph\xi_p\xi_h} \langle h\xi_h| \delta H(r) |p\xi_p\rangle + c_{ph\xi_p\xi_h} \langle p\xi_p| \delta H(r) |h\xi_h\rangle] \\ &= \sum_{ph\xi_p\xi_h} [c^*_{ph\xi_p\xi_h} \delta\tilde{h}(q,\xi_p\xi_h) + c_{ph\xi_p\xi_h} \delta\tilde{h}^*(q,\xi_p\xi_h)] \end{aligned} \tag{B.2}$$

Usually we assume $\delta\tilde{h}(q,\xi_p\xi_h)$ to be real. We should again here take a look at the mean value of V

$$\begin{aligned}
\langle\Psi(t)|\,V\,|\Psi(t)\rangle = \frac{1}{2}\sum_{\substack{\alpha\beta\gamma\delta\\ \xi_\alpha\xi_\beta\xi_\gamma\xi_\delta}} &\langle\alpha\beta\xi_\alpha\xi_\beta|\,V\,|\gamma\delta\xi_\gamma\xi_\delta\rangle \\
&\langle\Psi_0|\,(1+\sum_{ph\xi_p\xi_h} c^*_{ph\xi_p\xi_h}a^\dagger_{h\xi_h}a_{p\xi_p}+\frac{1}{2}(\sum_{ph\xi_p\xi_h} c^*_{ph\xi_p\xi_h}a^\dagger_{h\xi_h}a_{p\xi_p})^2)(a^\dagger_{\alpha\xi_\alpha}a^\dagger_{\beta\xi_\beta}a_{\delta\xi_\delta}a_{\gamma\xi_\gamma}) \\
&(1+\sum_{p'h'\xi_{p'}\xi_{h'}} c_{p'h'\xi_{p'}\xi_{h'}}a^\dagger_{p'\xi_{p'}}a_{h'\xi_{h'}}+\frac{1}{2}(\sum_{p'h'\xi_{p'}\xi_{h'}} c_{p'h'\xi_{p'}\xi_{h'}}a^\dagger_{p'\xi_{p'}}a_{h'\xi_{h'}})^2)\,|\Psi_0\rangle \\
&= \sum_{\substack{pp'hh'\\ \xi_p\xi_{p'}\xi_h\xi_{h'}}} \Big(\left\langle ph'\xi_p\xi_{h'}\right|V\left|hp'\xi_h\xi_{p'}\right\rangle_a c^*_{ph\xi_p\xi_h}c_{p'h'\xi_{p'}\xi_{h'}} \\
&+\frac{1}{2}\left\langle pp'\xi_p\xi_{p'}\right|V\left|hh'\xi_h\xi_{h'}\right\rangle_a c^*_{ph\xi_p\xi_h}c^*_{p'h'\xi_{p'}\xi_{h'}} \\
&+\frac{1}{2}\left\langle hh'\xi_h\xi_{h'}\right|V\left|pp'\xi_p\xi_{p'}\right\rangle_a c_{ph\xi_p\xi_h}c_{p'h'\xi_{p'}\xi_{h'}}\Big)
\end{aligned} \tag{B.3}$$

Using RPA we neglect the exchange interaction, then by variational method we can get the interaction part of the TDHF equations

$$\frac{\partial\langle V\rangle}{\partial c^*} = \sum_{p'h'\xi_{p'}\xi_{h'}}\Big(\left\langle ph'\xi_p\xi_{h'}\right|V\left|hp'\xi_h\xi_{p'}\right\rangle c_{p'h'\xi_{p'}\xi_{h'}}+\left\langle pp'\xi_p\xi_{p'}\right|V\left|hh'\xi_h\xi_{h'}\right\rangle c^*_{p'h'\xi_{p'}\xi_{h'}}\Big) \tag{B.4}$$

$$\frac{\partial\langle V\rangle}{\partial c} = \sum_{p'h'\xi_{p'}\xi_{h'}}\Big(\left\langle hp'\xi_h\xi_{p'}\right|V\left|ph'\xi_p\xi_{h'}\right\rangle c^*_{p'h'\xi_{p'}\xi_{h'}}+\left\langle hh'\xi_h\xi_{h'}\right|V\left|pp'\xi_p\xi_{p'}\right\rangle c_{p'h'\xi_{p'}\xi_{h'}}\Big) \tag{B.5}$$

c has the form

$$c(t) = xe^{-i\omega t}+y^*e^{i\omega t} \tag{B.6}$$

We can write the above 2 formulas as

$$\sum_{p'h'\xi_{p'}\xi_{h'}}\Big(\left\langle ph'\xi_p\xi_{h'}\right|V\left|hp'\xi_h\xi_{p'}\right\rangle x_{p'h'\xi_{p'}\xi_{h'}}+\left\langle pp'\xi_p\xi_{p'}\right|V\left|hh'\xi_h\xi_{h'}\right\rangle y_{p'h'\xi_{p'}\xi_{h'}}\Big) \tag{B.7}$$

$$\sum_{p'h'\xi_{p'}\xi_{h'}}\Big(\left\langle hh'\xi_h\xi_{h'}\right|V\left|pp'\xi_p\xi_{p'}\right\rangle x_{p'h'\xi_{p'}\xi_{h'}}+\left\langle hp'\xi_h\xi_{p'}\right|V\left|ph'\xi_p\xi_{h'}\right\rangle y_{p'h'\xi_{p'}\xi_{h'}}\Big) \tag{B.8}$$

For spin-orbit coupling, we have $V = V_{LS}(r)\mathbf{r}_{12} \times \mathbf{p}_{12} \cdot \boldsymbol{\sigma}_{12}$ with $\boldsymbol{\sigma}_{12} = \boldsymbol{\sigma}_1 + \boldsymbol{\sigma}_2$Then we can write the two equations as

$$\sum_{p'h'\xi_{p'}\xi_{h'}} \Big(\left\langle ph' \right| V_{LS}(r)\mathbf{r}_{12} \times \mathbf{p}_{12} \left| hp' \right\rangle \cdot \left\langle \xi_p \xi_{h'} \right| \boldsymbol{\sigma}_{12} \left| \xi_h \xi_{p'} \right\rangle x_{p'h'\xi_{p'}\xi_{h'}} + \left\langle pp' \right| V_{LS}(r)\mathbf{r}_{12} \times \mathbf{p}_{12} \left| hh' \right\rangle \cdot \left\langle \xi_p \xi_{p'} \right| \boldsymbol{\sigma}_{12} \left| \xi_h \xi_{h'} \right\rangle y_{p'h'\xi_{p'}\xi_{h'}} \Big) \tag{B.9}$$

$$\sum_{p'h'\xi_{p'}\xi_{h'}} \Big(\left\langle hh' \right| V_{LS}(r)\mathbf{r}_{12} \times \mathbf{p}_{12} \left| pp' \right\rangle \cdot \left\langle \xi_h \xi_{h'} \right| \boldsymbol{\sigma}_{12} \left| \xi_p \xi_{p'} \right\rangle x_{p'h'\xi_{p'}\xi_{h'}} + \left\langle hp' \right| V_{LS}(r)\mathbf{r}_{12} \times \mathbf{p}_{12} \left| ph' \right\rangle \cdot \left\langle \xi_h \xi_{p'} \right| \boldsymbol{\sigma}_{12} \left| \xi_p \xi_{h'} \right\rangle y_{p'h'\xi_{p'}\xi_{h'}} \Big) \tag{B.10}$$

We have evaluated that

$$\left\langle ph' \right| V_{LS}(r)\mathbf{r}_{12} \times \mathbf{p}_{12} \left| hp' \right\rangle = \frac{\mathrm{i}}{2N} \frac{\partial \tilde{V}_{LS}}{\partial q} \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \delta(\mathbf{q} - \mathbf{q}') \tag{B.11}$$

$$\left\langle pp' \right| V_{LS}(r)\mathbf{r}_{12} \times \mathbf{p}_{12} \left| hh' \right\rangle = \frac{\mathrm{i}}{2N} \frac{\partial \tilde{V}_{LS}}{\partial q} \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \delta(\mathbf{q} + \mathbf{q}') \tag{B.12}$$

Also

$$\sum_{h'} \mathbf{h}' x_{h'-q,h,\xi_{h'-q}\xi_{h'}} = -\sum_{h'} \mathbf{h}' x_{h'+q,h',\xi_{h'+q}\xi_{h'}} \tag{B.13}$$

Therefore we can write our TDHF equations as, forcing $\mathbf{p}' = \mathbf{h}' + \mathbf{q}$

$$(\varepsilon_p - \varepsilon_h - \omega) x_{ph\xi_p\xi_h} + \frac{\mathrm{i}}{2N} \frac{\partial \tilde{V}_{LS}}{\partial q} \sum_{h'\xi_{p'}\xi_{h'}} \Big[\hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \cdot \left\langle \xi_p \xi_{h'} \right| \boldsymbol{\sigma}_{12} \left| \xi_h \xi_{p'} \right\rangle x_{p'h'\xi_{p'}\xi_{h'}} + \hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}') \cdot \left\langle \xi_p \xi_{p'} \right| \boldsymbol{\sigma}_{12} \left| \xi_h \xi_{h'} \right\rangle y_{p'h'\xi_{p'}\xi_{h'}} \Big] + \delta\tilde{h}(q, \xi_p \xi_h) = 0 \tag{B.14}$$

$$(\varepsilon_p - \varepsilon_h + \omega) y_{ph\xi_p\xi_h} - \frac{\mathrm{i}}{2N} \frac{\partial \tilde{V}_{LS}}{\partial q} \sum_{h'\xi_{p'}\xi_{h'}} \Big[\hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}') \cdot \left\langle \xi_h \xi_{h'} \right| \boldsymbol{\sigma}_{12} \left| \xi_p \xi_{p'} \right\rangle x_{p'h'\xi_{p'}\xi_{h'}} + \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \cdot \left\langle \xi_h \xi_{p'} \right| \boldsymbol{\sigma}_{12} \left| \xi_p \xi_{h'} \right\rangle y_{p'h'\xi_{p'}\xi_{h'}} \Big] + \delta\tilde{h}(q, \xi_p \xi_h) = 0 \tag{B.15}$$

Now we have to show all the matrix elements of $\boldsymbol{\sigma}_{12}$ in the basis of $\left|\uparrow\uparrow\right\rangle, \left|\uparrow\downarrow\right\rangle, \left|\downarrow\uparrow\right\rangle, \left|\downarrow\downarrow\right\rangle$.

$$\boldsymbol{\sigma}_{12} = \begin{pmatrix} 2\hat{z} & \hat{x} - \mathrm{i}\hat{y} & \hat{x} - \mathrm{i}\hat{y} & 0 \\ \hat{x} + \mathrm{i}\hat{y} & 0 & 0 & \hat{x} - \mathrm{i}\hat{y} \\ \hat{x} + \mathrm{i}\hat{y} & 0 & 0 & \hat{x} - \mathrm{i}\hat{y} \\ 0 & \hat{x} + \mathrm{i}\hat{y} & \hat{x} + i\hat{y} & -2\hat{z} \end{pmatrix} \tag{B.16}$$

We should write down all the TDHF equations for all elements of the spin matrix. For $\xi_p = \uparrow, \xi_h = \uparrow$

$$(\varepsilon_p - \varepsilon_h - \omega)x_{ph\uparrow\uparrow} + \frac{\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}\sum_{h'}\big[\hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \cdot (2\hat{z}x_{p'h'\uparrow\uparrow} + (\hat{x} + \mathrm{i}\hat{y})x_{p'h'\uparrow\downarrow} + (\hat{x} - \mathrm{i}\hat{y})x_{p'h'\downarrow\uparrow}) \\ + \hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}') \cdot (2\hat{z}y_{p'h'\uparrow\uparrow} + (\hat{x} - \mathrm{i}\hat{y})y_{p'h'\uparrow\downarrow} + (\hat{x} + \mathrm{i}\hat{y})y_{p'h'\downarrow\uparrow})\big] + + \delta\tilde{h}(q, \uparrow\uparrow) = 0 \tag{B.17}$$

$$(\varepsilon_p - \varepsilon_h + \omega)y_{ph\uparrow\uparrow} - \frac{\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}\sum_{h'}\big[\hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}') \cdot (2\hat{z}x_{p'h'\uparrow\uparrow} + (\hat{x} - \mathrm{i}\hat{y})x_{p'h'\uparrow\downarrow} + (\hat{x} + \mathrm{i}\hat{y})x_{p'h'\downarrow\uparrow}) \\ + \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \cdot (2\hat{z}y_{p'h'\uparrow\uparrow} + (\hat{x} + \mathrm{i}\hat{y})y_{p'h'\uparrow\downarrow} + (\hat{x} - \mathrm{i}\hat{y})y_{p'h'\downarrow\uparrow})\big] + + \delta\tilde{h}(q, \uparrow\uparrow) = 0 \tag{B.18}$$

For $\xi_p = \downarrow, \xi_h = \downarrow$

$$(\varepsilon_p - \varepsilon_h - \omega)x_{ph\downarrow\downarrow} + \frac{\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}\sum_{h'}\big[\hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \cdot (-2\hat{z}x_{p'h'\downarrow\downarrow} + (\hat{x} + \mathrm{i}\hat{y})x_{p'h'\uparrow\downarrow} + (\hat{x} - \mathrm{i}\hat{y})x_{p'h'\downarrow\uparrow}) \\ + \hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}') \cdot (-2\hat{z}y_{p'h'\downarrow\downarrow} + (\hat{x} - \mathrm{i}\hat{y})y_{p'h'\uparrow\downarrow} + (\hat{x} + \mathrm{i}\hat{y})y_{p'h'\downarrow\uparrow})\big] + + \delta\tilde{h}(\downarrow\downarrow) = 0 \tag{B.19}$$

$$(\varepsilon_p - \varepsilon_h + \omega)y_{ph\downarrow\downarrow} - \frac{\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}\sum_{h'}\big[\hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}') \cdot (-2\hat{z}x_{p'h'\downarrow\downarrow} + (\hat{x} - \mathrm{i}\hat{y})x_{p'h'\uparrow\downarrow} + (\hat{x} + \mathrm{i}\hat{y})x_{p'h'\downarrow\uparrow}) \\ + \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}') \cdot (-2\hat{z}y_{p'h'\downarrow\downarrow} + (\hat{x} + \mathrm{i}\hat{y})y_{p'h'\uparrow\downarrow} + (\hat{x} - \mathrm{i}\hat{y})y_{p'h'\downarrow\uparrow})\big] + + \delta\tilde{h}(q, \downarrow\downarrow) = 0 \tag{B.20}$$

We can combine these 4 equations into 2 as

$$x_{ph\uparrow\uparrow} + x_{ph\downarrow\downarrow} = -\frac{1}{\varepsilon_p - \varepsilon_h - \omega}\left\{\frac{\mathrm{i}}{N}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}} \times \left[\sum_{h'}(\mathbf{h} - \mathbf{h}') \cdot \sum_{\xi_{p'}\xi_{h'}} \langle \xi_{h'} | \boldsymbol{\sigma} | \xi_{p'} \rangle x_{p'h'\xi_{p'}\xi_{h'}} \right.\right. \\ \left.\left. + \sum_{h'}(\mathbf{h} + \mathbf{h}') \cdot \sum_{\xi_{p'}\xi_{h'}} \langle \xi_{p'} | \boldsymbol{\sigma} | \xi_{h'} \rangle y_{p'h'\xi_{p'}\xi_{h'}} \right] + \delta\tilde{h}(q, \uparrow\uparrow) + \delta\tilde{h}(q, \downarrow\downarrow)\right\} \tag{B.21}$$

$$y_{ph\uparrow\uparrow} + y_{ph\downarrow\downarrow} = -\frac{1}{\varepsilon_p - \varepsilon_h + \omega}\left\{\frac{-\mathrm{i}}{N}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{\mathbf{q}} \times \left[\sum_{h'}(\mathbf{h} + \mathbf{h}') \cdot \sum_{\xi_{p'}\xi_{h'}} \langle \xi_{h'} | \boldsymbol{\sigma} | \xi_{p'} \rangle x_{p'h'\xi_{p'}\xi_{h'}} \right.\right. \\ \left.\left. + \sum_{h'}(\mathbf{h} - \mathbf{h}') \cdot \sum_{\xi_{p'}\xi_{h'}} \langle \xi_{p'} | \boldsymbol{\sigma} | \xi_{h'} \rangle y_{p'h'\xi_{p'}\xi_{h'}} \right] + \delta\tilde{h}(q, \uparrow\uparrow) + \delta\tilde{h}(q, \downarrow\downarrow)\right\} \tag{B.22}$$

Here $\boldsymbol{\sigma}$ is the single-particle spin matrix which has the form

$$\boldsymbol{\sigma} = \begin{pmatrix} \hat{z} & \hat{x} - \mathrm{i}\hat{y} \\ \hat{x} + \mathrm{i}\hat{y} & -\hat{z} \end{pmatrix} \tag{B.23}$$

And we can see

$$\sum_{\xi_p\xi_h} \langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\, x_{ph\xi_p\xi_h} = \hat{z}x_{ph\uparrow\uparrow} + (\hat{x}+\mathrm{i}\hat{y})x_{ph\uparrow\downarrow} + (\hat{x}-\mathrm{i}\hat{y})x_{ph\downarrow\uparrow} - \hat{z}x_{ph\downarrow\downarrow} \tag{B.24}$$

$$\sum_{\xi_p\xi_h} \langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\, y_{ph\xi_p\xi_h} = \hat{z}y_{ph\uparrow\uparrow} + (\hat{x}-\mathrm{i}\hat{y})y_{ph\uparrow\downarrow} + (\hat{x}+\mathrm{i}\hat{y})y_{ph\downarrow\uparrow} - \hat{z}y_{ph\downarrow\downarrow} \tag{B.25}$$

Here we hope to evaluate the expressions of $\sum_h(\sum_{\xi_p\xi_h}\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\, x_{ph\xi_p\xi_h} + \sum_{\xi_p\xi_h}\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\, y_{ph\xi_p\xi_h})$ and $\sum_h \hat{\mathbf{q}}\times\mathbf{h}(\sum_{\xi_p\xi_h}\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\, x_{ph\xi_p\xi_h} - \sum_{\xi_p\xi_h}\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\, y_{ph\xi_p\xi_h})$ in terms of $\sum_h(x_{ph\uparrow\uparrow} + \tilde{x}_{ph\downarrow\downarrow} + y_{\uparrow\uparrow} + y_{\downarrow\downarrow}$ so that we can get the linear response expression of the sum of diagonal elements. Looking back to the 4 equations of $\xi_P=\uparrow, \xi_h=\uparrow$ and $\xi_p=\downarrow, \xi_h=\downarrow$, we can combine them by substraction as

$$\begin{aligned} x_{ph\uparrow\uparrow} - x_{ph\downarrow\downarrow} = -\frac{1}{\varepsilon_p-\varepsilon_h-\omega}\Bigg\{\sum_{h'}\frac{\mathrm{i}}{N}\frac{\partial\tilde{V}_{LS}}{\partial q}\hat{z}\cdot\big[\hat{\mathbf{q}}\times(\mathbf{h}-\mathbf{h}')(x_{ph\uparrow\uparrow}+x_{ph\downarrow\downarrow}) \\ +\hat{\mathbf{q}}\times(\mathbf{h}+\mathbf{h}')(y_{ph\uparrow\uparrow}+y_{ph\downarrow\downarrow})\big] + \delta\tilde{h}(q,\uparrow\uparrow) - \delta\tilde{h}(q,\downarrow\downarrow)\Bigg\} \end{aligned} \tag{B.26}$$

$$\begin{aligned} y_{ph\uparrow\uparrow} - y_{ph\downarrow\downarrow} = -\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\Bigg\{\sum_{h'}\frac{-\mathrm{i}}{N}\frac{\partial\tilde{V}_{LS}}{\partial q}\hat{z}\cdot\big[\hat{\mathbf{q}}\times(\mathbf{h}+\mathbf{h}')(x_{ph\uparrow\uparrow}+x_{ph\downarrow\downarrow}) \\ +\hat{\mathbf{q}}\times(\mathbf{h}-\mathbf{h}')(y_{ph\uparrow\uparrow}+y_{ph\downarrow\downarrow})\big] + \delta\tilde{h}(q,\uparrow\uparrow) - \delta\tilde{h}(q,\downarrow\downarrow)\Bigg\} \end{aligned} \tag{B.27}$$

If we are careful enough, we can see that

$$x_{ph\uparrow\uparrow} - x_{ph\downarrow\downarrow} = \sum_{\xi_p\xi_h}\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\cdot\hat{z}x_{ph\xi_p\xi_h} \tag{B.28}$$

$$y_{ph\uparrow\uparrow} - y_{ph\downarrow\downarrow} = \sum_{\xi_p\xi_h}\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\cdot\hat{z}y_{ph\xi_p\xi_h} \tag{B.29}$$

$$\begin{aligned} \delta\tilde{h}(q,\uparrow\uparrow) - \delta\tilde{h}(q,\downarrow\downarrow) &= \sum_{\xi_p\xi_h}\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\cdot\hat{z}\delta\tilde{h}(q,xi_p\xi_h) \\ &= \sum_{\xi_p\xi_h}\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\cdot\hat{z}\delta\tilde{h}(q,xi_p\xi_h) \end{aligned} \tag{B.30}$$

Now we can take a look at the non-diagonal term $\xi_p =\uparrow, \xi_h =\downarrow$ and $\xi_p =\downarrow, \xi_h =\uparrow$, which give 4 equations

$$x_{ph\uparrow\downarrow} = -\frac{1}{\varepsilon_p - \varepsilon_h - \omega}\left\{\sum_{h'} \frac{\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}(\hat{x} - \mathrm{i}\hat{y}) \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] + \delta\tilde{h}(q, \uparrow\downarrow)\right\} \quad (B.31)$$

$$x_{ph\downarrow\uparrow} = -\frac{1}{\varepsilon_p - \varepsilon_h - \omega}\left\{\sum_{h'} \frac{\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}(\hat{x} + \mathrm{i}\hat{y}) \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] + \delta\tilde{h}(q, \downarrow\uparrow)\right\} \quad (B.32)$$

$$y_{ph\uparrow\downarrow} = -\frac{1}{\varepsilon_p - \varepsilon_h + \omega}\left\{\sum_{h'} \frac{-\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}(\hat{x} - \mathrm{i}\hat{y}) \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] + \delta\tilde{h}(q, \uparrow\downarrow)\right\} \quad (B.33)$$

$$y_{ph\downarrow\uparrow} = -\frac{1}{\varepsilon_p - \varepsilon_h + \omega}\left\{\sum_{h'} \frac{-\mathrm{i}}{2N}\frac{\partial \tilde{V}_{LS}}{\partial q}(\hat{x} + \mathrm{i}\hat{y}) \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] + \delta\tilde{h}(q, \downarrow\uparrow)\right\} \quad (B.34)$$

Now we can play around these 4 equations to get the other two components in $\hat{x}$ and $\hat{y}$ directions of $\sum_{\xi_p\xi_h} \langle\xi_h|\boldsymbol{\sigma}|\xi_p\rangle x_{ph\xi_p\xi_h}$ and $\sum_{\xi_p\xi_h} \langle\xi_p|\boldsymbol{\sigma}|\xi_h\rangle y_{ph\xi_p\xi_h}$. In $\hat{x}$ direction

$$x_{ph\uparrow\downarrow} + x_{ph\downarrow\uparrow} = -\frac{1}{\varepsilon_p - \varepsilon_h - \omega}\left\{\sum_{h'} \frac{\mathrm{i}}{N}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{x} \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] + \delta\tilde{h}(q, \uparrow\downarrow) + \delta\tilde{h}(q, \downarrow\uparrow)\right\} \quad (B.35)$$

$$y_{ph\uparrow\downarrow} + y_{ph\downarrow\uparrow} = -\frac{1}{\varepsilon_p - \varepsilon_h + \omega}\left\{\sum_{h'} \frac{-\mathrm{i}}{N}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{x} \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] + \delta\tilde{h}(q, \uparrow\downarrow) + \delta\tilde{h}(q, \downarrow\uparrow)\right\} \quad (B.36)$$

In $\hat{x}$ direction

$$\mathrm{i}x_{ph\uparrow\downarrow} - \mathrm{i}x_{ph\downarrow\uparrow} = -\frac{i}{\varepsilon_p - \varepsilon_h - \omega}\left\{\sum_{h'} \frac{1}{N}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{y} \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] + \delta\tilde{h}(q, \uparrow\downarrow) - \delta\tilde{h}(q, \downarrow\uparrow)\right\} \quad (B.37)$$

$$-\mathrm{i}y_{ph\uparrow\downarrow} + \mathrm{i}y_{ph\downarrow\uparrow} = -\frac{i}{\varepsilon_p - \varepsilon_h + \omega}\left\{\sum_{h'} \frac{1}{N}\frac{\partial \tilde{V}_{LS}}{\partial q}\hat{y} \cdot \left[\hat{\mathbf{q}} \times (\mathbf{h} + \mathbf{h}')(x_{p'h'\uparrow\uparrow} + x_{p'h'\downarrow\downarrow}) \right.\right.$$
$$\left.\left. + \hat{\mathbf{q}} \times (\mathbf{h} - \mathbf{h}')(y_{p'h'\uparrow\uparrow} + y_{p'h'\downarrow\downarrow})\right] - \delta\tilde{h}(q, \uparrow\downarrow) + \delta\tilde{h}(q, \downarrow\uparrow)\right\} \quad (B.38)$$

Base on all these 3 components, we can conclude that

$$\begin{aligned}
&\frac{1}{N}\sum_{h\xi_p\xi_h}\left(\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\, x_{ph\xi_p\xi_h}+\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\, y_{ph\xi_p\xi_h}\right)\\
=&-\frac{1}{N}\sum_{h}\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}-\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\hat{\mathbf{q}}\times\mathbf{h})\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'}(x_{p'h'\uparrow\uparrow}+x_{p'h'\downarrow\downarrow}+y_{p'h'\uparrow\uparrow}+y_{p'h'\downarrow\downarrow})\\
&+\frac{1}{N}\sum_{h}\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'}\hat{\mathbf{q}}\times\mathbf{h}'(x_{p'h'\uparrow\uparrow}+x_{p'h'\downarrow\downarrow}-y_{p'h'\uparrow\uparrow}-y_{p'h'\downarrow\downarrow})\\
&-\frac{1}{N}\sum_{h\xi_p\xi_h}\left(\frac{\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle}{\varepsilon_p-\varepsilon_h-\omega}+\frac{\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle}{\varepsilon_p-\varepsilon_h+\omega}\right)\delta\tilde{h}(q,\xi_p\xi_h)
\end{aligned}\tag{B.39}$$

We have proven that

$$\sum_h\frac{1}{\varepsilon_p-\varepsilon_h\pm\omega}(\hat{\mathbf{q}}\times\mathbf{h})=0\tag{B.40}$$

So the first term on the right hand side of eq.(B.39) vanishes. Here we can get another equation

$$\begin{aligned}
&\frac{1}{N}\sum_{h\xi_p\xi_h}(\hat{\mathbf{q}}\times\mathbf{h})\cdot\left(\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\, x_{ph\xi_p\xi_h}-\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\, y_{ph\xi_p\xi_h}\right)\\
=&-\frac{1}{N}\sum_{h}\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\hat{\mathbf{q}}\times\mathbf{h})^2\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'}(x_{p'h'\uparrow\uparrow}+x_{p'h'\downarrow\downarrow}+y_{p'h'\uparrow\uparrow}+y_{p'h'\downarrow\downarrow})\\
&+\frac{1}{N}\sum_{h}\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}-\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\\
&(\hat{\mathbf{q}}\times\mathbf{h})\cdot\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'}\hat{\mathbf{q}}\times\mathbf{h}'(x_{p'h'\uparrow\uparrow}+x_{p'h'\downarrow\downarrow}-y_{p'h'\uparrow\uparrow}-y_{p'h'\downarrow\downarrow})\\
&-\frac{1}{N}\sum_{h\xi_p\xi_h}(\hat{\mathbf{q}}\times\mathbf{h})\cdot\left(\frac{\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle}{\varepsilon_p-\varepsilon_h-\omega}-\frac{\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle}{\varepsilon_p-\varepsilon_h+\omega}\right)\delta\tilde{h}(q,\xi_p\xi_h)
\end{aligned}\tag{B.41}$$

Base on the same reason, we can say that the second term and the third term on the RHS of eq.(B.41) vanish. Now we can combine eq.(B.21) and eq.(B.22) to get

$$\begin{aligned}
&\frac{1}{N}\sum_h (x_{ph\uparrow\uparrow}+x_{ph\downarrow\downarrow}+y_{ph\uparrow\uparrow}+y_{ph\downarrow\downarrow}) = -\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}-\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\\
&(\hat{\mathbf{q}}\times\mathbf{h})\cdot\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'\xi_{p'}\xi_{h'}}(\langle\xi'_h|\boldsymbol{\sigma}|\xi'_p\rangle x_{p'h'\xi'_p\xi'_h}+\langle\xi'_p|\boldsymbol{\sigma}|\xi'_h\rangle y_{p'h'\xi'_p\xi'_h})\\
&+\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\\
&\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'\xi_{p'}\xi_{h'}}(\hat{\mathbf{q}}\times\mathbf{h}')(\langle\xi'_h|\boldsymbol{\sigma}|\xi'_p\rangle x_{p'h'\xi'_p\xi'_h}-\langle\xi'_p|\boldsymbol{\sigma}|\xi'_h\rangle y_{p'h'\xi'_p\xi'_h})\\
&-\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\delta\tilde{h}(q,\uparrow\uparrow)+\delta\tilde{h}(q,\downarrow\downarrow))
\end{aligned} \tag{B.42}$$

We can again argue that the first term vanishes. Substitute eq.(B.41) to this equation we get

$$\begin{aligned}
&\frac{1}{N}\sum_h (x_{ph\uparrow\uparrow}+x_{ph\downarrow\downarrow}+y_{ph\uparrow\uparrow}+y_{ph\downarrow\downarrow}) = +\left(\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\right)\\
&\left(\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\hat{\mathbf{q}}\times\mathbf{h})^2\right)\left(\frac{\partial\tilde{V}_{LS}}{\partial q}\right)^2\\
&\frac{1}{N}\sum_{h'}(x_{p'h'\uparrow\uparrow}+x_{p'h'\downarrow\downarrow}+y_{p'h'\uparrow\uparrow}+y_{p'h'\downarrow\downarrow})\\
&-\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\delta\tilde{h}(q,\uparrow\uparrow)+\delta\tilde{h}(q,\downarrow\downarrow))
\end{aligned} \tag{B.43}$$

Define

$$\chi_0 = -\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right) \tag{B.44}$$

$$\chi'_0 = -\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\hat{\mathbf{q}}\times\mathbf{h})^2 \tag{B.45}$$

We can get the linear response equation

$$\sum_{\xi=\uparrow\uparrow,\downarrow\downarrow}(\tilde{x}(q,\xi)+\tilde{y}(q,\xi)) = \frac{\chi_0}{1-\left(\frac{\partial\tilde{V}_{LS}}{\partial q}\right)^2\chi_0\chi'_0}\sum_{\xi=\uparrow\uparrow,\downarrow\downarrow}\delta\tilde{h}(q,\xi) \tag{B.46}$$

This is the linear response equation for the sum of all diagonal terms. Fortunately it's just the same as what I have derived previously(there was a sign problem in the denominator of the response function, after correcting that it is the same as this one). To achieve this, we need to take a closer look at eq.(B.39), excluding the vanishing term

$$\begin{aligned}&\frac{1}{N}\sum_{h\xi_p\xi_h}\left(\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\, x_{ph\xi_p\xi_h}+\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\, y_{ph\xi_p\xi_h}\right)\\ =&\frac{1}{N}\sum_{h}\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'}\hat{\mathbf{q}}\times\mathbf{h}'(x_{p'h'\uparrow\uparrow}+x_{p'h'\downarrow\downarrow}-y_{p'h'\uparrow\uparrow}-y_{p'h'\downarrow\downarrow})\\ &-\frac{1}{N}\sum_{h\xi_p\xi_h}\left(\frac{\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle}{\varepsilon_p-\varepsilon_h-\omega}+\frac{\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle}{\varepsilon_p-\varepsilon_h+\omega}\right)\delta\tilde{h}(q,\xi_p\xi_h)\end{aligned}\tag{B.47}$$

If we use vector analysis, the left hand side should be in the same direction as the right hand side, which means the first term of the RHS should be in the direction of $\boldsymbol{\sigma}$. This is an important argument to extract the non-diagonal sum. Now we can combine eq.(B.21) and eq.(B.22) again to get an equation, excluding the vanishing terms, as

$$\begin{aligned}&\frac{1}{N}\hat{\mathbf{q}}\times\mathbf{h}\sum_h(x_{ph\uparrow\uparrow}+x_{ph\downarrow\downarrow}-y_{ph\uparrow\uparrow}-y_{ph\downarrow\downarrow})=\\ &-\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\hat{\mathbf{q}}\times\mathbf{h})\\ &\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'\xi_{p'}\xi_{h'}}(\hat{\mathbf{q}}\times\mathbf{h})\cdot\left(\langle\xi'_h|\,\boldsymbol{\sigma}\,|\xi'_p\rangle\, x_{p'h'\xi'_p\xi'_h}+\langle\xi'_p|\,\boldsymbol{\sigma}\,|\xi'_h\rangle\, y_{p'h'\xi'_p\xi'_h}\right)\end{aligned}\tag{B.48}$$

Let $\mathbf{a}=\hat{\mathbf{q}}\times\mathbf{h}$, and we know that

$$(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{a}\cdot\boldsymbol{\sigma})=\mathbf{a}^2+i\mathbf{a}\times\mathbf{a}\cdot\boldsymbol{\sigma}=\mathbf{a}^2\tag{B.49}$$

Therefore

$$\mathbf{a}(\mathbf{a}\cdot\boldsymbol{\sigma})=\mathbf{a}^2\boldsymbol{\sigma}+(\text{perpendicular to }\boldsymbol{\sigma})\tag{B.50}$$

As we have discussed that the LHS of eq.(B.48) is in the direction of $\boldsymbol{\sigma}$, it's better to believe that the perpendicular part will at least cancel out after the sum, so that we can rewrite

$$(\hat{\mathbf{q}}\times\mathbf{h})((\hat{\mathbf{q}}\times\mathbf{h})\cdot\boldsymbol{\sigma})=(\hat{\mathbf{q}}\times\mathbf{h})^2\boldsymbol{\sigma}\tag{B.51}$$

And eq.(B.48) is

$$\begin{aligned}&\frac{1}{N}\hat{\mathbf{q}}\times\mathbf{h}\sum_h(x_{ph\uparrow\uparrow}+x_{ph\downarrow\downarrow}-y_{ph\uparrow\uparrow}-y_{ph\downarrow\downarrow})=\\ &-\frac{1}{N}\sum_h\left(\frac{1}{\varepsilon_p-\varepsilon_h-\omega}+\frac{1}{\varepsilon_p-\varepsilon_h+\omega}\right)(\hat{\mathbf{q}}\times\mathbf{h})^2\\ &\mathrm{i}\frac{\partial\tilde{V}_{LS}}{\partial q}\frac{1}{N}\sum_{h'\xi_{p'}\xi_{h'}}\left(\langle\xi'_h|\,\boldsymbol{\sigma}\,|\xi'_p\rangle\, x_{p'h'\xi'_p\xi'_h}+\langle\xi'_p|\,\boldsymbol{\sigma}\,|\xi'_h\rangle\, y_{p'h'\xi'_p\xi'_h}\right)\end{aligned}\tag{B.52}$$

Put this back to eq.(B.47), we get

$$\begin{aligned}&\frac{1}{N}\sum_{h\xi_p\xi_h}\left(\langle\xi_h|\,\boldsymbol{\sigma}\,|\xi_p\rangle\,x_{ph\xi_p\xi_h}+\langle\xi_p|\,\boldsymbol{\sigma}\,|\xi_h\rangle\,y_{ph\xi_p\xi_h}\right)\\ =&\chi_0\left(\frac{\partial\tilde{V}_{LS}}{\partial q}\right)^2\chi_0'\frac{1}{N}\sum_{h'\xi_p'\xi_h'}\left(\langle\xi_h'|\,\boldsymbol{\sigma}\,|\xi_p'\rangle\,x_{p'h'\xi_p'\xi_h'}+\langle\xi_p'|\,\boldsymbol{\sigma}\,|\xi_h'\rangle\,y_{p'h'\xi_p'\xi_h'}\right)\\ &+\chi_0\boldsymbol{\sigma}\delta\tilde{h}(q,\xi_p\xi_h)\end{aligned} \tag{B.53}$$

And we can see the linear response equation of another channel is

$$\sum_h\boldsymbol{\sigma}(x_{ph\xi_p\xi_h}+y_{ph\xi_p\xi_h})=\frac{\chi_0}{1-\left(\frac{\partial\tilde{V}_{LS}}{\partial q}\right)^2\chi_0\chi_0'}\boldsymbol{\sigma}\delta\tilde{h}(q,\xi) \tag{B.54}$$

Here we eventually need a scalar form since our response function is a scalar. For the non-diagonal terms we have only σ_x components, which turns out to be

$$\sum_h(x_{ph\uparrow\downarrow}+y_{ph\downarrow\uparrow}+x_{ph\downarrow\uparrow}+y_{ph\uparrow\downarrow})=\frac{\chi_0}{1-\left(\frac{\partial\tilde{V}_{LS}}{\partial q}\right)^2\chi_0\chi_0'}[\delta\tilde{h}(q,\uparrow\downarrow)+\delta\tilde{h}(q,\downarrow\uparrow)] \tag{B.55}$$

It's a surprise that if we sum over both diagonal and non-diagonal terms, we will get

$$\sum_{h\xi_h\xi_p}(x_{ph\xi_p\xi_h}+y_{ph\xi_p\xi_h})=\frac{\chi_0}{1-\left(\frac{\partial\tilde{V}_{LS}}{\partial q}\right)^2\chi_0\chi_0'}\sum_\xi\delta\tilde{h}(q,\xi) \tag{B.56}$$

And it is exactly the same as our previous derivation.

Bibliography

[1] A.K Kerman and S.E Koonin. Hamiltonian formulation of time-dependent variational principles for the many-body system. *Annals of Physics*, 100(1):332 – 358, 1976. ISSN 0003-4916. doi: https://doi.org/10.1016/0003-4916(76)90065-8. URL http://www.sciencedirect.com/science/article/pii/0003491676900658.

[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Microscopic Theory of Superconductivity. *Physical Review*, 106:162–164, April 1957. doi: 10.1103/PhysRev.106.162.

[3] Yuan Cao, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, and Pablo Jarillo-Herrero. Unconventional superconductivity in magic-angle graphene superlattices. *NATURE*, 556(7699):43+, APR 5 2018. ISSN 0028-0836. doi: {10.1038/nature26160}.

[4] Richard A. Ferrell. Time-dependent hartree-fock theory of nuclear collective oscillations. *Phys. Rev.*, 107:1631–1634, Sep 1957. doi: 10.1103/PhysRev.107.1631. URL https://link.aps.org/doi/10.1103/PhysRev.107.1631.

[5] A. D. McLACHLAN and M. A. BALL. Time-dependent hartree—fock theory for molecules. *Rev. Mod. Phys.*, 36:844–855, Jul 1964. doi: 10.1103/RevModPhys.36.844. URL https://link.aps.org/doi/10.1103/RevModPhys.36.844.